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Asteroid identification using statistical orbital inversion methods

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Academic dissertation

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Cover:

Observed topocentric positions of moving objects and selected, realistic paths linking the positions. The observations were made in 2004 with the European Southern Observatory's Very Large Telescope (VLT) and the Canada-France-Hawaii Telescope (CFHT). The VLT observations were made on five consecutive nights (January 20-24; red, green, blue, magenta, and aqua), whereas the CFHT observations were made on January 22 (yellow) and January 30 (black). Each dot correspond to the first observation of an intrinsically correctly linked set of observations obtained at a single telescope during a single night. The linkages were found by using the methods presented in this thesis (Papers II and III).

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Abstract

An efficient and statistically robust solution for the identification of asteroids among numerous sets of astrometry is presented. In particular, numerical methods have been developed for the short-term identification of asteroids at discovery, and for the long-term identification of scarcely observed asteroids over apparitions, a task which has been lacking a robust method until now. The methods are based on the solid foundation of statistical orbital inversion properly taking into account the observational uncertainties, which allows for the detection of practically all correct identifications. Through the use of dimensionality-reduction techniques and efficient data structures, the exact methods have a loglinear, that is, $\mathcal{O}(n \log n)$, computational complexity, where n is the number of included observation sets. The methods developed are thus suitable for future large-scale surveys which anticipate a substantial increase in the astrometric data rate.

Due to the discontinuous nature of asteroid astrometry, separate sets of astrometry must be linked to a common asteroid from the very first discovery detections onwards. The reason for the discontinuity in the observed positions is the rotation of the observer with the Earth as well as the motion of the asteroid and the observer about the Sun. Therefore, the aim of identification is to find a set of orbital elements that reproduce the observed positions with residuals similar to the inevitable observational uncertainty. Unless the astrometric observation sets are linked, the corresponding asteroid is eventually lost as the uncertainty of the predicted positions grows too large to allow successful follow-up.

Whereas the presented identification theory and the numerical comparison algorithm are generally applicable, that is, also in fields other than astronomy (e.g., in the identification of space debris), the numerical methods developed for asteroid identification can immediately be applied to all objects on heliocentric orbits with negligible effects due to non-gravitational forces in the time frame of the analysis.

The methods developed have been successfully applied to various identification problems. Simulations have shown that the methods developed are able to find virtually all correct linkages despite challenges such as numerous scarce observation sets, astrometric uncertainty, numerous objects confined to a limited region on the celestial sphere, long linking intervals, and substantial parallaxes. Tens of previously unknown main-belt asteroids have been identified with the short-term method in a preliminary study to locate asteroids among numerous unidentified sets of single-night astrometry of moving objects, and scarce astrometry obtained nearly simultaneously with Earth-based and space-based telescopes has been successfully linked despite a substantial parallax. Using the long-term method, thousands of realistic 3-linkages typically spanning several apparitions have so far been found among designated observation sets each spanning less than 48 hours.

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List of papers

- I Granvik, M., Virtanen J., Muinonen, K., Bowell, E., Koehn, B., and Tancredi, G. 2003. Transneptunian Object Ephemeris Service (TNOEPH). *Earth, Moon and Planets* **92**, 73–78.
- II Granvik, M., and Muinonen, K. 2005. Asteroid identification at discovery. *Icarus* **179**, 1, 109–127.
- III Granvik, M., Muinonen, K., Jones, L., Bhattacharya, B., Delbó, M., Saba, L., Cellino, A., Tedesco, E. F., Davis, D. R., and Meadows, V. 2007. Linking Large-Parallax Spitzer-CFHT-VLT Astrometry of Asteroids. *Icarus*, in press.
- IV Muinonen, K., Virtanen, J., Granvik, M., and Laakso, T. 2006. Asteroid orbits using phase-space volumes of variation. *MNRAS*, **368**, 2, 809–818.
- V Granvik, M., and Muinonen, K. 2007. Near-Earth-Object Identification Over Apparitions Using n -body Ranging. In *Near Earth Objects, our Celestial Neighbors: Opportunity and Risk* (A. Milani, G. B. Valsecchi, and D. Vokrouhlický, Eds.), pp. 281–290. Cambridge University Press, Cambridge, UK.
- VI Granvik, M., and Muinonen, K. 2007. Asteroid identification over apparitions. *Icarus*, submitted.

Acronyms and abbreviations used in the text

AU Astronomical Unit

CFHT Canada-France-Hawaii Telescope

ESA European Space Agency

ESO European Southern Observatory

CCD Charge Coupled Device

Dec. Declination

JPL Jet Propulsion Laboratory

LOV Line Of Variation

LSL Least Squares with Linearization

MAC Multiple-Address Comparison

MBO Main-Belt Object

MC Monte Carlo

MPC Minor Planet Center

NEO Near-Earth Object

$O - C$ Observed minus Computed (residuals)

Pan-STARRS Panoramic Survey Telescope And Rapid Response System

p.d.f. Probability-Density Function

R.A. Right Ascension

RB tree Red-Black tree

rms Root Mean Square

TNO Transneptunian Object

VLT Very Large Telescope

VoV Volume Of Variation

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1 Introduction

The linking of asteroid astrometry, that is, the identification of asteroids in the observational data, precedes all further analysis of the objects. The successful linking leads to a decreased orbital uncertainty, due to the increase in usually both the total observational time span and the number of observations. The unsuccessful linking, on the other hand, may ultimately lead to the underlying asteroid being lost, because the uncertainty of predicted positions increases as a function of the time interval between the last observation date and the prediction date. Identification can therefore be seen as an essential part of asteroid discovery (cf. Milani et al. 2007).

The discontinuity of asteroid astrometry typically arises due to reasons stemming both from the geometry of the Sun-Moon-observatory-asteroid quadruple and the light-scattering properties of the asteroid. Whereas the rotation of the Earth results in gaps between nightly observation sets, the brightness of the full Moon often prevents the detection of faint objects and thus groups the observations into different *lunations*.

Observations are also intercepted because of asteroids being visible only because they reflect the sunlight incident on them. First, the apparent brightness of an asteroid depends on its distance from the Sun so that, as the distance grows, the asteroid becomes fainter, and vice versa. Second, the brightness also depends on the Sun-asteroid-observer angle called the phase angle. The brightness reaches its maximum for zero phase angle, that is, at opposition. Discarding the reasons for the shorter gaps in the data, the increasing brightness of an asteroid around opposition makes it continuously observable for a period of time, which is called the *apparition* (cf. opposition).

Typically, the time interval between two successive apparitions depends on the synodic period between the Earth and the asteroid. For a main-belt object (MBO) the typical time interval between the mid-apparition dates is 15 months, while for a transneptunian object (TNO) the typical time interval is one year due to the large heliocentric distance as compared to the Earth. Near-Earth objects (NEOs) have a wide variety of different time intervals, mainly due to the complicated and quickly changing mutual geometry of the Sun, the asteroid, and the Earth. Long time intervals, say, several years, can be imagined either for comet-like or Earth-like orbits. While an NEO on a comet-like orbit with a high eccentricity only makes short visits to the near-Earth region, NEOs on Earth-like orbits stay in the near-Earth region but have an unfavorable location close to, or even behind, the Sun for relatively long periods of time.

As the motion of the solar-system object requires the linking of the separate observation sets in the first place, the solution to the linking problem is an orbit which reproduces the observed astrometry with an accuracy similar to the ob-

servational uncertainty. The most important input data for orbit computation is classical astrometry (hereafter referred to as astrometry), that is, the sky-plane coordinates Right Ascension (R.A.) and Declination (Dec.) measured on different dates. The other types of astrometry, time-delay and Doppler obtained with radar, measure coordinates in the radial direction. Radar astrometry is therefore orthogonal to classical astrometry measuring the transverse coordinates.

In principle, the linking problem could also be solved using other types of data. It is often suggested that asteroid photometry could also be used. Unfortunately, the uncertainties associated with contemporary photometry, obtained by professional asteroid surveys and amateurs alike, are too large to allow us to discard linkages based on the usually small differences in the observed brightnesses. Moreover, the rotation of an asteroid results in a time-dependent brightness variation which can have an amplitude of, say, one magnitude unit. For recently discovered asteroids, the shape and surface characteristics are not known well enough to allow photometry to be an important source of data for linking methods. However, photometry can be used to discard linkages showing anomalously large brightness variations.

The identification process becomes computationally challenging, when the asteroid is hidden among numerous scarce (astrometric) data sets, each of which is internally correctly linked. Particularly from the point of view of the impending next-generation asteroid surveys, promising an unprecedented asteroid discovery rate, the simplistic identification methods used so far become impractical. Whereas the conventional methods have a computational complexity of $\mathcal{O}(n^2)$ (hereafter referred to as quadratic methods), n being the number of data sets, the increasing discovery rate requires identification methods with a computational complexity of $\mathcal{O}(n \log n)$ (hereafter referred to as loglinear methods). When the work on the present thesis began, two challenging identification problems were essentially unsolved. Hereafter they are referred to as the short-term and long-term problems (cf. Muinonen & Bowell 1993).

In the short-term problem, numerous sets of scarce single-night astrometry, which cannot be identified as belonging to previously known objects, are confined to a limited region on the celestial sphere and have been obtained over a relatively short period of time, say, days or weeks. The scenario is typical for dedicated asteroid surveys but, mostly due to the relatively low discovery rate, it has not been considered particularly problematic until recent years. However, from the point of view of the impending next-generation asteroid surveys the methods used so far become impractical. During the last few years, two groups have therefore developed and published loglinear methods for the short-term problem (in addition to the present thesis, see, Kubica 2005).

The most challenging long-term problem only emerges for a fraction of the de-

tected asteroids. The orbital uncertainties for some asteroids remain large, because they have only been observed during one or two nights without proper follow-up. An asteroid lacking proper follow-up can be “rediscovered”—typically it is not apparent that the object has already been discovered and therefore it receives an additional designation—at subsequent apparitions, e.g., several years later, and, in the worst-case scenario, is lost again before proper follow-up can be obtained to allow the linkage to the earlier apparition. However, by locating and combining the scarce data sets of the same asteroid obtained at different apparitions, the orbital uncertainty can be reduced and the asteroid can be removed from the list of lost objects. As of January 1, 2007 roughly 54,000 provisionally designated sets of astrometry—approximately 15% of the $\sim 365,000$ solar-system small bodies then known—span less than 48 hours, which means that the majority of them are essentially lost. In the current thesis, I present the first robust method to search for linkages between scarce sets of astrometry spanning only a day or two. Being loglinear, the method is also suitable for future needs.

A few remarks are in place on the terminology adopted. An *identification* usually implies the same as a *linkage*. The difference is that objects are identified while observation sets are linked. Note that the two terms used have a related though different meaning in connection to asteroid families and in the search for parent bodies for meteorites. Here, a linkage, or an identification, means that an orbital solution exists which reproduces the observed positions within observational uncertainties. To emphasize that the solution to the present linking problem must be able to reproduce the astrometry, the problem should actually be called the *astrometric linking problem*. However, throughout the thesis, the term *astrometric* has been omitted. The definition of *scarce* data should here be understood as an amount of observations spanning such a short time that the resulting orbital-element probability-density function (p.d.f.) is non-Gaussian. In practice, this means that the orbit-computation methods used cannot assume a Gaussian p.d.f., and the orbital-element p.d.f. must therefore be sampled to obtain a rigorous estimate for the orbital uncertainty. For the Gaussian assumption to be valid, the number of observations and the length of the observational time span—the latter of which usually is the more important one—must typically be determined on a case-by-case basis. The terms *object* or *body* are used as synonyms for *asteroid* to emphasize that the distinction between asteroids and comets is all but evident according to our current understanding. Where the objects under study have been called asteroids, it has usually been done to stress that non-gravitational forces typical for comets have not been treated. Unless otherwise stated, the term *observation* is used as a synonym for the classic astrometric observation, that is, an R.A. and Dec. pair. The *sensitivity* is defined as the ratio of the number of correct linkages found and the number of correct linkages present. Note that the value of

the latter is exactly known only for simulated data. The *positive-predictive value* is the fraction of the number of correct linkages found and the number of all linkages found.

The thesis consists of the following papers:

Paper I Granvik, M., Virtanen J., Muinonen, K., Bowell, E., Koehn, B., and Tancredi, G. 2003. Transneptunian Object Ephemeris Service (TNOEPH). *Earth, Moon and Planets* **92**, 73–78.

Paper II Granvik, M., and Muinonen, K. 2005. Asteroid identification at discovery. *Icarus* **179**, 1, 109–127.

Paper III Granvik, M., Muinonen, K., Jones, L., Bhattacharya, B., Delbó, M., Saba, L., Cellino, A., Tedesco, E. F., Davis, D. R., and Meadows, V. 2007. Linking Large-Parallax Spitzer-CFHT-VLT Astrometry of Asteroids. *Icarus*, in press.

Paper IV Muinonen, K., Virtanen, J., Granvik, M., and Laakso, T. 2006. Asteroid orbits using phase-space volumes of variation. *MNRAS*, **368**, 2, 809–818.

Paper V Granvik, M., and Muinonen, K. 2007. Near-Earth-Object Identification Over Apparitions Using *n*-body Ranging. In *Near Earth Objects, our Celestial Neighbors: Opportunity and Risk* (A. Milani, G. B. Valsecchi, and D. Vokrouhlický, Eds.), pp. 281–290. Cambridge University Press, Cambridge, UK.

Paper VI Granvik, M., and Muinonen, K. 2007. Asteroid identification over apparitions. *Icarus*, submitted.

Paper I presents a web service based on statistical orbital ranging (Ranging; Virtanen et al. 2001, Muinonen et al. 2001) for the identification of TNO precovery observations as well as the planning of TNO follow-up observations. Simultaneously, the service can also be used as a verification tool for TNO identifications over apparitions: if an orbital solution can be found for astrometry combined of two or more separate data sets using realistic astrometric uncertainties, the observation sets can be linked. Paper II presents a new linking method which is optimized for the short-term linking problem and is based on Ranging. Paper III continues the topic of Paper II, and presents a case study of a particularly challenging short-term linking problem involving substantial parallaxes, numerous scarce data sets, and a high sky-plane density of objects. Whereas Ranging is optimized for scarce data sets, a new six-dimensional sampling method for the inversion of moderate asteroid astrometry for the orbital-element p.d.f. is presented in Paper IV. Paper V generalizes Ranging by completely removing the dynamical two-body approximation

from the analysis. Finally, Paper VI presents a new—and so far the only—method for the linking of scarce asteroid astrometry over apparitions.

The thesis is organized as follows. Chapter 2 describes the background for the present thesis. The different populations of small solar-system bodies are described in Section 2.1. Challenges for the impending next-generation surveys—rising from the nature of the observed populations—are also outlined. As a historical background, the early advances in asteroid identification are reviewed in Section 2.2, whereas Section 2.3 reviews more recent alternative solutions to the identification problem. Statistical orbit computation is reviewed in Chapter 3, and the numerical techniques used in the papers of this thesis are summarized. Chapter 4 describes and discusses the theoretical and numerical solutions to the asteroid identification problem relying on statistical orbital inversion, and Section 4.3 presents selected results obtained with the methods developed. Summaries of the papers of the thesis are given in Chapter 5. Conclusions and future prospects are offered in Chapter 6. Finally, the thesis is brought to a closure with Papers I–VI.

2 Asteroids and their identification

2.1 Surveying the solar system

Asteroids are divided into separate populations based on their Keplerian orbital elements—semimajor axis a , eccentricity e , inclination i , longitude of the ascending node Ω , argument of perihelion ω , and mean anomaly M_0 —and the resulting perihelion distance $q = a(1-e)$ and aphelion distance $Q = a(1+e)$ given for a specified epoch t_0 . Starting from the Sun, the most frequently discussed populations are NEOs, Mars-crossers, Hungarias, MBOs, Cybeles, Hildas, Jupiter Trojans, Centaurs, and TNOs. Moreover, a population barely discovered, with only a few accepted members, is expected to be located completely interior to the Earth’s orbit—hence the name inner-Earth objects (IEOs). Although the definitions of different asteroid populations are under constant debate, rough locations of the populations in the orbital-element phase space can be given (Table 1).

Asteroid populations			
Population	Bounds on		
	a	q	Q
IEO	—	—	$Q < q_{\oplus}$
NEO	—	$q < 1.3 \text{ AU}$	$Q > q_{\oplus}$
Mars-crosser	—	$1.3 \text{ AU} < q < Q_{\odot}$	$Q > q_{\odot}$
Hungaria	$1.8 \text{ AU} < a < 2 \text{ AU}$	$q > Q_{\odot}$	—
MBO	$2.2 \text{ AU} < a < 3.3 \text{ AU}$	$q > Q_{\odot}$	—
Cybele	$3.3 \text{ AU} < a < 3.7 \text{ AU}$	—	—
Hilda	$3.7 \text{ AU} < a < 4.2 \text{ AU}$	—	—
Jovian Trojan	$4.8 \text{ AU} < a < 5.2 \text{ AU}$	$q > 4.2 \text{ AU}$	—
Centaur	$5.5 \text{ AU} < a < 30 \text{ AU}$	$q > 5.2 \text{ AU}$	—
TNO	$a > a_{\Psi}$	—	—

Table 1: Approximate bounds for various asteroid populations in the (a, q, Q) -space. $q_{\oplus} \approx 0.983 \text{ AU}$ is the perihelion distance of the Earth, $Q_{\odot} \approx 1.67 \text{ AU}$ is the aphelion distance for Mars, and $a_{\Psi} \approx 30.3 \text{ AU}$ is the semimajor axis of Neptune. Hildas are in a 3:2 mean-motion resonance with Jupiter. Jovian Trojans are in a 1:1 mean-motion resonance with Jupiter and are located in two separate groups centered roughly 60° ahead of and behind the planet.

During the last two decades, the public in general and politicians in the United States (U.S.) in particular have become aware of the risk posed by asteroid and comet impacts to the Earth. The increased awareness has created a network of mostly U.S.-government-funded surveys dedicated to the search for NEOs, the

potential impactors. According to a mandate issued by the U.S. Congress in 1998, 90% of NEOs larger than 1 km in diameter, which roughly equals an absolute magnitude $H \lesssim 18$ mag, were to be discovered within a ten-year period. Asteroids larger than 1 km in diameter are capable of causing a global catastrophe in a collision with the Earth, and their discovery and follow-up was therefore deemed an appropriate goal. The five NEO surveys currently online, and also responsible for most of the NEO discoveries so far, are the University of Arizona Lunar and Planetary Laboratory’s (UA/LPL) Spacewatch group, Jet Propulsion Laboratory’s (JPL) Near-Earth Asteroid Tracking (NEAT), Lowell Observatory Near-Earth-Object Search (LONEOS), Lincoln Laboratory’s Near Earth Asteroid Research (LINEAR) program, and UA/LPL’s Catalina Sky Survey (CSS). For details and comparisons between the active NEO surveys, see Stokes et al. (2002) and the recent review by Larson (2007). Although focusing on NEOs, the surveys have substantially increased our knowledge of all asteroid populations. In addition to the dedicated NEO searches, other types of surveys also collect observational data on asteroids. For example, the Sloan Digital Sky Survey (SDSS), although primarily focusing on galaxies, has detected tens of thousands of solar-system objects, a fraction of which belong to new discoveries (Ivezić et al. 2001). Another example is Lowell Observatory’s Deep Ecliptic Survey (DES) aiming for the discovery of TNOs (see, e.g., Millis et al. 2002).

The (a, e, i) -distribution of selected objects as of August 22, 2007 are shown in Fig. 1. All above-mentioned populations can be distinguished, although the known IEO population currently only includes a few members. Most asteroids currently known have low-eccentricity orbits close to the ecliptic plane. Kirkwood gaps (Kirkwood 1867) caused by strong planetary resonances can be discerned in the main belt. Due to the resonances—most of which are too weak to clean up their neighborhood and show up as gaps in the (a, e) -plane—and other weaker forces such as the Yarkovsky force (see, e.g., review by Bottke et al. 2002b), the small-body populations are constantly evolving. Objects from the outskirts of the solar system move inwards, and eventually end their journey in the solar system either by colliding with the Sun or the terrestrial planets or by being thrown out from the solar system via a close approach to Jupiter.

Based on the then-known asteroid populations and the characteristics of the surveys mostly responsible for the discoveries, Jedicke et al. (2002) gave debiased estimations for the size distributions of different asteroid populations. Fig. 2 shows the size distributions as estimated by Jedicke et al. (2002) together with the currently known populations deriving from the ASTORB database (Bowell et al. 1994) dated 22 August, 2007. Although we currently know almost 380,000 objects, there is significantly more to be discovered. For example, even if the Centaur population is estimated to contain a substantial fraction of the total mass of the solar-system

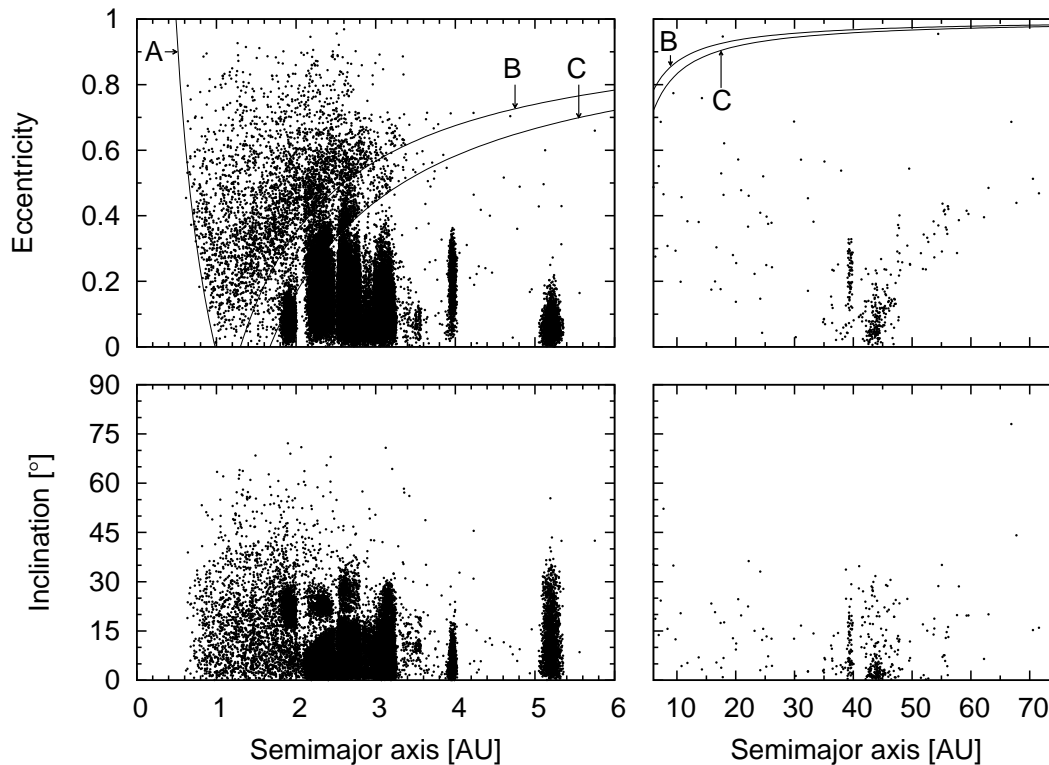


Figure 1: Distribution of a , e and i for most of the known asteroids as of August 22, 2007. Plots to the left portray the inner solar system ($0 \text{ AU} < a < 6 \text{ AU}$), whereas plots to the right present the outer solar system ($6 \text{ AU} < a < 75 \text{ AU}$). The upper plots show the eccentricity versus the semimajor axis, and the lower plots the inclination versus the semimajor axis. A, B, and C mark the lines for $Q = q_{\oplus} = 0.983 \text{ AU}$, $q = 1.3 \text{ AU}$, and $q = Q_{\odot} = 1.67 \text{ AU}$, respectively. The orbits for 297,075 objects observed for more than three weeks ($q < 1.3 \text{ AU}$), more than three months ($q > 1.3 \text{ AU}$ and $a < 5.5 \text{ AU}$), or more than three years ($q > 1.3 \text{ AU}$ and $a > 5.5 \text{ AU}$) were obtained from the ASTORB database (Bowell et al. 1994) dated August 22, 2007. Note that only every tenth MBO orbit fulfilling the criteria is plotted, and that the semimajor axis and inclination distributions have artificial cutoffs at 75 AU and 90° , respectively.

small bodies, it is one of the least observed asteroid populations with only few tens of known members. Note that the size of the largest object in each population is typically proportional to the average heliocentric distance of that population.

As the ten-year period of the congressional mandate issued in 1998 is soon ending and the surveys have more or less met the goal, another congressional mandate has set a new target. The next plan is to discover 90% of all NEOs larger than 140 m, or $H < 22 \text{ mag}$, by the year 2020. Whereas the previous goal is being met with dedicated surveys having limiting magnitudes ranging from 18.9 mag to

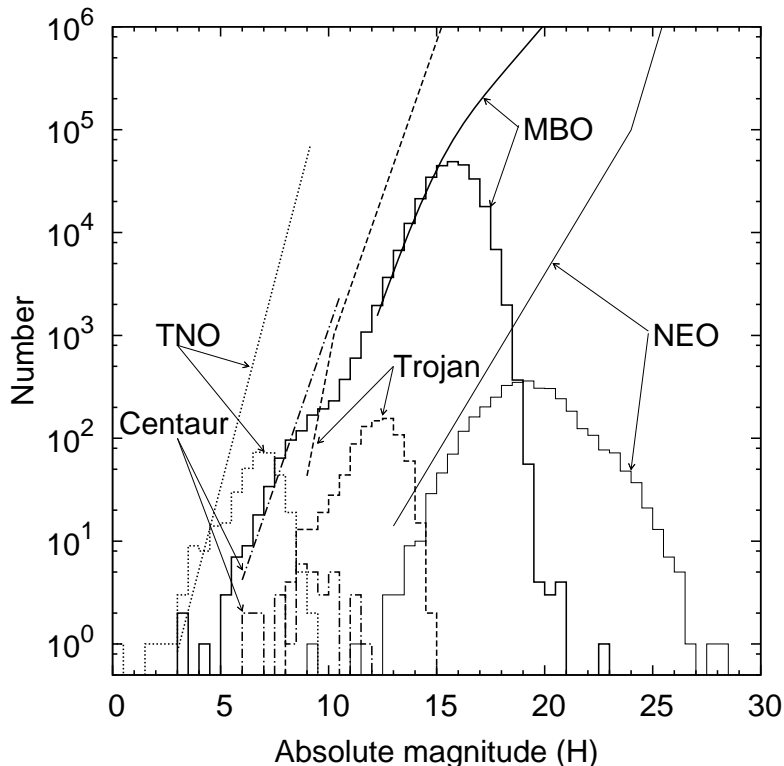


Figure 2: Estimated and observed size distributions for different asteroid populations. Assuming a geometric albedo of 0.15, an absolute magnitude of $H = 5$ mag corresponds to an asteroid diameter of approximately 350 km, whereas an absolute magnitude of $H = 25$ mag corresponds to a diameter of a few tens of meters. The estimated size distributions (lines) have been derived by Jedicke et al. (2002) and the observed size distributions (histograms) have been obtained from the ASTORB database (Bowell et al. 1994) with the criteria given in the caption of Fig. 1.

22.0 mag (Larson 2007), the planned, and partially built, next-generation surveys such as, e.g., the Panoramic Survey Telescope And Rapid Response System (Pan-STARRS; the prototype of which is coming online in 2008; Jedicke et al. 2007), the Discovery Channel Telescope (DCT; first light in late 2009 or early 2010; Bowell et al. 2007), and the Large Synoptic Survey Telescope (LSST; first light possibly in 2013; Ivezić et al. 2007), have to reach considerably fainter magnitudes to meet the goal. The anticipated limiting magnitudes range from 24 mag to 25 mag. In addition to detecting fainter objects, the new surveys will also scan the visible sky considerably faster than the current surveys. As the number of asteroids increases exponentially with decreasing size (Fig. 2), the rate of asteroid discovery is expected to increase by up to two orders of magnitude from the current average of 100 discoveries per night to an average of 10,000 discoveries per night.

In addition to the ground-based surveys, the identification problem has to be solved for space-based surveys such as the one to be performed by Gaia (see, e.g., Muinonen et al. 2005, Mignard et al. 2007) during its nominal five-year mission starting in late 2011. It has been estimated that most of the $\sim 500,000$ asteroids to be detected by Gaia will be known, but some 10% can be new discoveries.

2.2 Early advances in asteroid identification

The first modern solution to an astrometric linking problem for small solar-system objects was presented by Anders Johan Lexell (1777). For reviews, see Valsecchi (2007) and Markkanen et al. (1984). Lexell linked two sets of comet astrometry, the first spanning approximately three weeks and the second spanning approximately eight weeks, over a gap of two months with a single elliptic orbit. The comet—discovered in 1770 by Charles Messier but now bearing the name D/1770 L1 Lexell or just Comet Lexell—turned out to be the first NEO found. According to Lexell’s calculations, a close encounter with Jupiter in 1767 had brought it to the inner solar system, and he also correctly predicted that due to another, even closer encounter with Jupiter in 1779, the comet’s perihelion distance would increase again and make it unobservable with the telescopes of that time. Prior to Lexell’s work, comet sightings had only been linked by comparing their approximate orbital characteristics derived from parabolic orbits. Observations between different apparitions had not been connected with a single set of orbital elements. Lexell was the first researcher to use Newtonian mechanics (Newton 1687) to compute an elliptic orbit which acceptably reproduced the observed positions for a small solar-system object.

The first asteroid, (1) Ceres, was discovered in January 1801 by Giuseppe Piazzi (see recent review by Foderá Serio et al. 2002). The circumstances of that discovery illustrate the challenges faced in the follow-up of recently discovered objects and, further, in the linking of scarce asteroid astrometry. Piazzi observed Ceres on 14 nights during a period of 23 days, but he did not report the discovery to other observers in time to allow for straightforward follow-up. As the orbit computation methods available at that time required a priori assumptions for the resulting orbit, for example, a circular orbit, it turned out to be impossible to compute ephemerides accurate enough to allow recovery. To allow more accurate ephemerides, the young mathematician Carl Friedrich Gauss developed the least-squares method to compute what is now known as the maximum-likelihood orbit by minimizing the square of the *Observed minus Computed* ($O - C$) residuals (Gauss 1809). By using the optimized orbit, Gauss computed predicted positions leading to the recovery of Ceres in December 1801 by Baron Franz Xaver von Zach.

Whereas the above-mentioned examples solely deal with the problem of finding a single orbit which reproduces the astrometry of either a single observation

set or combined observation sets, the first dedicated and systematic asteroid surveys in the early 1950's and 1960's highlighted the problem of identifying different asteroids among a wealth of scarce data sets. The McDonald Observatory asteroid survey (MDS; Kuiper et al. 1958) had a limiting photographic magnitude of 16.5 mag and covered the opposition-centered $40^\circ \times 40^\circ$ region for 23 consecutive lunations. MDS produced altogether 3,247 separate single-night sets of asteroid astrometry. Provisionally designated asteroids and numbered asteroids were identified in the data based on the approximate position (ephemeris uncertainty $\sim 1'$), the approximate daily motion and “the rough magnitude, although the latter was not very reliable.” The positions and motions of the known asteroids were computed for the observation dates from various ephemeris tables either graphically or by using “the second differences in the interpolation”. The positions computed were also allowed to vary along the line of variation. The astrometry of the objects, identified or not, located on two overlapping plates obtained during the same lunation, was linked by superimposing the plates and correcting for motion where necessary. The astrometry corresponding to unidentified objects obtained during different lunations was in some cases successfully linked by extrapolating the daily motion. However, 26% of the detected objects remained unidentified.

With a limiting photographic magnitude of 20.5 mag, the Palomar-Leiden survey (PLS; van Houten et al. 1970) measured altogether some 14,000 positions of more than 2,000 asteroids. The astrometry was obtained during two separate lunations with a gap of almost three weeks in between. During the first lunation, each field was covered with three plate pairs during a five day period. During the second lunation, the fields were also covered on three different nights, but the cadence was different with two plate pairs taken with an interval of two days and the third plate pair obtained a week earlier. For most objects detected, the total observational time span was approximately one month. Whereas the linking of the single-night sets within each lunation was satisfactorily performed by visually estimating both the brightness and the motion of an object, linking astrometry between the lunations led to “considerable difficulties.” Initially, the linkages were sought by extrapolating the arc from the first lunation to the second lunation by starting with the brightest object. Although most of the successful identifications were apparent immediately, many erroneous linkages were also made. For example, two data sets of the same object were erroneously linked to astrometry of other objects, and the correct identification could thus not be made. By computing orbital elements using the method by Herget (1965) and, further, search ephemerides, some erroneous linkages were rectified and a few new ones found. van Houten et al. (1970) considered orbital elements computed for data sets spanning five days to be unreliable, and they therefore resorted to the so-called Väisälä orbits (Väisälä 1939) which are based on the assumption that the object is at

perihelion. Using ephemerides computed from the Väisälä orbits and the so-called eccentricity-assumed orbits, van Houten et al. (1970) and van Houten et al. (1984), respectively, were able to make some additional linkages. However, a number of objects observed in PLS still remain unidentified.

Whereas the above-mentioned examples refer to identification work carried out as part of surveys, pure archive searches have also been carried out. For example, Schmadel (1982) compared the perturbed ephemerides of the first 2,297 numbered asteroids with the 43,076 then-unidentified observations, which resulted in 1,884 new identifications with 1,100 asteroids. For particularly interesting objects such as NEOs, it is, in some cases, possible to identify additional so-called precovery observations. Precovery observations have been obtained, but not measured, before the discovery of the object under consideration. By computing ephemerides corresponding to the observation dates of photographic plates or CCD images, additional, previously missed detections can be located (see, e.g., Boattini et al. 2001). The DLR-Archhold Near Earth Objects Precovery Survey (DANEOPS) has been a particularly successful project between amateurs (foremost A. Doppler and A. Gnädig) and professionals searching for precovery observations of NEOs and other interesting objects (see, e.g., Bowell et al. 2002).

2.3 Alternative approaches

Until recent years, asteroid identifications have mostly been and are partially still (private communication with E. Bowell and T. Spahr) sought among measured astrometric data sets using approaches which are often based on either linear extrapolations of the observed positions (see, e.g., Ivezić et al. 2001) or the so-called classical orbit-computation methods such as the Väisälä method (for a review on the traditional identification methods, see Marsden 1986). Particularly the Väisälä-based methods, although founded on approximations, have been successfully dealing with the data rate to the point that methods with a higher sensitivity have not been called for. Moreover, Marsden (1980) states that the “detective work involved in the establishment of identifications [of observations of a given asteroid at different apparitions] has played an important role in the study of minor planets ever since the early days of photography”, but “it has generally been conducted as a spare-time occupation.” Consequently, the development of new approaches to the identification of asteroids among numerous sets of astrometry also remained minuscule. Based on the published works primarily focusing on identification methods, the development of asteroid identification methods has been considered its own field of study only for the last two decades. As mentioned in Chapter 1, the currently rising interest for the identification methods is foremost due to the continuously increasing data rate of the dedicated NEO surveys which will eventually make the simplified approaches impractical.

Marsden (1985) gave examples of how the orbit linking two widely separated observation sets can be obtained with what he called the Gauss-Encke-Merton method or the Moulton-Väisälä-Cunningham method. He notes, however, that the methods used cannot always find the orbit linking observation sets. As the identification of meteor streams with similar orbits resembles the identification of asteroids using orbital elements, variants of the D -criterion originally published by Southworth & Hawkins (1963) for meteor stream identification have also been used in quadratic asteroid identification methods (see, e.g., Marsden 1986).

Milani (1999) presented the one-dimensional line-of-variation (LOV) method which maps the ridge of the non-Gaussian orbital-element p.d.f. with numerous “virtual asteroids”, and gave examples on how the method could find new identifications between asteroids. Milani et al. (2000) found linkages between provisionally designated data sets by searching for overlapping confidence ellipsoids (Milani & Valsecchi 1999) in the orbital-element phase space. The confidence ellipsoids were defined by the orbital-element covariance matrices obtained from the least-squares method. In an analysis including 35,121 sets of astrometry with at least four good observations spanning at least four days (two thirds of the sets spanned more than 20 days), their quadratic method lead to the identification of 152 asteroids with two different designations. Using another quadratic algorithm, Milani et al. (2001) identified scarce observation sets by requiring that the ephemeris-space confidence ellipsoid stemming from the least-squares orbit of a known asteroid includes the identified observations. During one year of operation the method had produced some 1,500 identifications accepted by the MPC.

Milani et al. (2004) defined what they termed the admissible region for a scarce observation set by combining a so-called attributable—the quartet of R.A. and Dec. with their time derivatives—and its covariance matrix (all obtained by computing a least-squares fit for the observed R.A. and Dec. values) with the (range, range rate)-plane of acceptable solutions, where the range is the topocentric distance r and the range rate the radial velocity \dot{r} . The space of acceptable solutions was analytically defined by requiring that the data set does not belong to a satellite of the Earth, does not belong to an object controlled by the Earth, belongs to a solar-system object, and belongs to an object outside the Earth. The (r, \dot{r}) -plane is sampled using Delaunay triangulation. The concept of admissible regions was applied to the short-term linking problem by Milani et al. (2005a). They presented a quadratic algorithm which requires a candidate linkage between three data sets, that is, a 3-linkage, before an orbital analysis can be performed. Whereas the method was tested only over intervals of four days, the authors speculated that the method could perform well even for 12-day intervals. Recently, Tommei et al. (2007) derived the analytical expressions for the admissible regions of space debris on geocentric orbits for both optical and radar astrometry. They also outlined a

quadratic identification algorithm for space debris.

In addition to reviews and results of the previous methods, Milani et al. (2005b, for another review, see also Sansaturio & Arratia 2007) presented an improved version of the quadratic identification method used in the orbital-element phase-space (Milani et al. 2000). They gave a definition for LOV different from that by Milani (1999). Following the new definition, a global least-squares solution need not exist, as initial orbital elements can be obtained through an educated guess for the new LOV method. According to the identifications accepted by the MPC, the new so-called constrained multiple-solution method has been proven to have a considerably higher sensitivity as compared to the previous methods.

Closely related to the Pan-STARRS project, Kubica et al. (2007, see also Kubica 2005) recently published a loglinear method for the linking of scarce asteroid astrometry over time intervals of up to a few weeks. Working in the observation space (R.A. and Dec.), they traverse all those paths between observed positions which can acceptably be fitted with a second-order polynomial. By using k -dimensional tree-like data structures, all the paths can be traversed in loglinear time. The approach by Kubica et al. (2007) has, through extensive simulations, proven to be particularly attractive for the linking of positions observed during the same night, that is, for intra-night linking. Whereas the approximations used limit the applicability of the method to linking observation sets over time intervals of, say, several weeks (cf. van Houten et al. 1970), the same approximations are well suited for intra-night linking due to the typically almost linear motion of an asteroid during a single night.

Kristensen (2007) reviews a suite of different methods that use a geometric approach to short-term linking. To the best of my knowledge, there does not exist published results of large-scale applications of the methods. The example cases only contain a few asteroids, which makes it impossible to estimate the sensitivities and positive-predictive values of the methods. Moreover, quadratic search algorithms and a fleet of assumptions (e.g., $a = 2.64$ AU, circular orbits) suggest that they are not applicable for the needs of the next-generation surveys that will detect a wide variety of objects on substantially different types of orbits (see also comments in Marsden 1991). For example, Pan-STARRS has a realistic chance of detecting interstellar visitors, or so-called orphan planets, on hyperbolic orbits with respect to the Sun (private communication with R. Jedicke). Missing important discoveries due to an overly simplified linking method is not acceptable for future large-scale surveys. In addition, it is interesting to note that in the above-mentioned, recent paper Kristensen writes: “Focus is on computational efficiency, so statistical (Monte Carlo) [identification] methods based on many orbits are excluded in advance.”

3 Statistical orbital inversion

3.1 Inverse theory

In orbit computation, the general *observation equation* describes the relation between observed positions and computed positions:

$$\boldsymbol{\psi} = \boldsymbol{\Psi}(\boldsymbol{P}) + \boldsymbol{\varepsilon} + \boldsymbol{\nu}. \quad (1)$$

The vector $\boldsymbol{\psi}$ contains the observed positions which are typically given as R.A. and Dec. pairs for the observation dates. \boldsymbol{P} contains the six orbital elements—usually Keplerian or Cartesian elements—at a specified epoch t_0 . The nonlinear function $\boldsymbol{\Psi}(\boldsymbol{P})$ gives the light-time-corrected topocentric positions computed from the orbital elements for the observation date. $\boldsymbol{\varepsilon}$ and $\boldsymbol{\nu}$ describe the random and systematic errors, respectively. For most modern applications, the systematic error is small enough to be incorporated into the typically much larger random error. In what follows, the systematic error is assumed negligible, that is, $\boldsymbol{\nu} = 0$.

The problem of computing positions $\boldsymbol{\Psi}$, that is, ephemerides, based on a set of orbital elements \boldsymbol{P} is called the *direct problem* of orbit computation. The *inverse problem* is to find the orbital elements \boldsymbol{P} given a set of observed positions $\boldsymbol{\psi}$. For the solution of both problems, a dynamical model is required. The model—typically based on Newtonian mechanics (Newton 1687) with a relativistic correction (Sitarski 1983) possibly added—is known with high accuracy. While the required parameters, such as masses and shapes of the perturbing bodies, are not always known accurately, the model and its parameters can safely be assumed exact given heliocentric, non-planet-approaching orbits and the typical observational uncertainties.

The geometric initial-orbit determination method as well as the least-squares method with linearized covariances (LSL)—both originally developed by Carl Friedrich Gauss (1809) in 1801 to find the then-lost asteroid Ceres—have remained the most extensively used orbital-inversion methods for nearly 200 years. While the previous method has evolved to several slightly different forms (see, e.g., Marsden 1985), the Gaussian assumptions—the observational errors follow a Gaussian distribution and the resulting orbital elements have a Gaussian p.d.f.—of the latter were not under debate for almost two centuries. Assuming the availability of a wealth of observed positions obtained at different observatories, the observational errors $\boldsymbol{\varepsilon}$ can safely be assumed Gaussian distributed according to the central limit theorem. If the data also spans a sufficiently long period of time, the linearization required for the computation of the covariance matrix in the least-squares method is applicable, and the orbital uncertainties given by the covariance matrix are valid. For NEOs, the rule of thumb is to have at least weeks of data before the Gaussian assumption can safely be assumed valid, while for MBOs and TNOs

the time spans are months and years, or even tens of years, respectively. However, before enough data has been collected, the orbital uncertainties cannot be rigorously expressed with the linearized covariance matrix. The non-Gaussian features of the orbit computation problem were studied by Muinonen & Bowell (1993), who laid the foundation for the statistical inversion of asteroid astrometry for the exact orbital-element p.d.f. and paved the way for non-Gaussian methods which do not expect the resulting orbital-element p.d.f.s to be Gaussian. In what follows, I will shortly present the statistical, or Bayesian, approach. For a more thorough review on the current status of asteroid orbital inversion, I refer the reader to the work by Virtanen (2005).

In the statistical inverse theory (see, e.g., Lehtinen 1988, and references therein), the (a posteriori) orbital-element p.d.f. p_p is proportional to the a priori (p_{pr}) and observational error (p_ϵ) p.d.f.s:

$$p_p(\mathbf{P}) = C p_{pr}(\mathbf{P}) p_\epsilon(\Delta\psi(\mathbf{P})). \quad (2)$$

$C = (\int p(\mathbf{P}, \psi) d\mathbf{P})^{-1}$ is the normalization constant, where the joint p.d.f. is $p(\mathbf{P}, \psi) = p_{pr}(\mathbf{P}) p_\epsilon(\Delta\psi(\mathbf{P}))$. Whereas p_ϵ is evaluated for the $O - C$ residuals $\Delta\psi(\mathbf{P})$ and is usually assumed to be Gaussian due to the above-mentioned central limit theorem, Muinonen & Bowell (1993) experimented with non-Gaussian noise statistics. They concluded that a significant improvement in the results, outweighing the more cumbersome analysis, could not be obtained.

To secure the invariance of the orbital-element p.d.f. p_p in transformations between different types of orbital elements (e.g., from Keplerian to Cartesian), the analysis is regularized by Jeffreys' a priori p.d.f. $p_{pr,J}$ (Jeffreys 1946):

$$\begin{aligned} p_{pr,J}(\mathbf{P}) &\propto \sqrt{\det \Sigma^{-1}(\mathbf{P})}, \\ \Sigma^{-1}(\mathbf{P}) &= \Phi(\mathbf{P})^T \Lambda^{-1} \Phi(\mathbf{P}), \end{aligned} \quad (3)$$

where Σ^{-1} is the information matrix evaluated for the local orbital elements \mathbf{P} , Φ contains the partial derivatives of the observed coordinates (usually R.A. and Dec.) with respect to the orbital elements, and Λ is the covariance matrix for the observational errors. Finally, the a posteriori orbital-element p.d.f. is given by

$$\begin{aligned} p_p(\mathbf{P}) &\propto \sqrt{\det \Sigma^{-1}(\mathbf{P})} \exp \left[-\frac{1}{2} \chi^2(\mathbf{P}) \right], \\ \chi^2(\mathbf{P}) &= (\Delta\psi(\mathbf{P}))^T \Lambda^{-1} \Delta\psi(\mathbf{P}). \end{aligned} \quad (4)$$

The a posteriori p.d.f. p_p can also include an informative a priori p.d.f. $p_{pr,inf}$, which is included as a separate factor in Eq. (4)

$$p_p(\mathbf{P}) \propto p_{pr,inf}(\mathbf{P}) \sqrt{\det \Sigma^{-1}(\mathbf{P})} \exp \left[-\frac{1}{2} \chi^2(\mathbf{P}) \right]. \quad (5)$$

The informative a priori p.d.f. can, for example, be used to set constraints on the a posteriori p.d.f. (Paper VI), or to combine inversion results obtained for different observation sets (an orbital-element p.d.f. computed from radar observations as an a priori p.d.f. for the inverse problem of optical astrometry, or vice versa).

The orbital-element p.d.f. p_p obtained can be transformed to the joint p.d.f. of any other parameter set ($\mathbf{F}(\mathbf{P}) = (F_1(\mathbf{P}), \dots, F_K(\mathbf{P}))^T$) by the following relation given in Muinonen & Bowell (1993):

$$p(\mathbf{F}) = \int d\mathbf{P} p_p(\mathbf{P}) \delta_D(F_1 - F_1(\mathbf{P})) \dots \delta_D(F_K - F_K(\mathbf{P})), \quad (6)$$

where δ_D is Dirac's delta function. For example, Eq. (6) can be used to transform the orbital-element p.d.f. from one set of elements to another (e.g., from Keplerian elements to Cartesian elements), or to propagate the orbital-element p.d.f. to the ephemerides p.d.f. (cf. Papers I-II).

In the future, when combining ground-based astrometry with astrometry from high-precision astrometry missions such as Gaia, the systematic error $\boldsymbol{\nu}$ here omitted may become relevant for the detection of interesting phenomena such as the photocenter-barycenter shift and the Yarkovsky effect (Mignard et al. 2007).

3.2 Numerical methods

For the inversion of asteroid astrometry for the orbital-element p.d.f., three different methods are used depending on the amount of available data. From scarce data, the orbital-element p.d.f. is obtained with Ranging (Virtanen et al. 2001, Muinonen et al. 2001) which samples the orbital-element p.d.f. in the following way:

- Two observations are chosen (usually the first and the last), and angular deviations mimicking the observational errors in R.A. and Dec. are introduced.
- Topocentric distances (or ranges) are assumed corresponding to the observation dates. By combining the topocentric positions with the heliocentric locations of the observatory at the observation dates, two heliocentric positions equaling six constants of integration are known.
- A trial orbit is solved from the two heliocentric positions and is then compared to all observations. If the trial orbit reproduces the observed positions to a predefined accuracy (defined as the relative-weight threshold c_{\min} and maximum sky-plane residuals of 3σ , where σ is the standard deviation of the assumed Gaussian observational error), it is added to the sample of possible orbits.

The relative weight c is defined as

$$c = \sqrt{\frac{\det \Sigma^{-1}(\mathbf{P})}{\det \Sigma^{-1}(\mathbf{P}_{\text{ref}})}} \exp \left[-\frac{1}{2}(\chi^2(\mathbf{P}) - \chi^2(\mathbf{P}_{\text{ref}})) \right] \quad (7)$$

where \mathbf{P}_{ref} refers to the best-fit orbital solution available, constantly updated during the iterative computation, and \mathbf{P} refers to the orbital elements of the sample orbit. For Gaussian p.d.f.s, $\chi^2(\mathbf{P}) - \chi^2(\mathbf{P}_{\text{ref}})$ becomes analogous to the $\Delta\chi^2$ defined as

$$\Delta\chi^2 = (\mathbf{P} - \mathbf{P}_{\text{ref}})^T \Sigma_{\text{ref}}^{-1} (\mathbf{P} - \mathbf{P}_{\text{ref}}). \quad (8)$$

In the basic version of Ranging, the initial topocentric distance intervals are determined manually using an educated guess, whereas in the automated version the topocentric distance intervals are further improved using the $3\text{-}\sigma$ cutoff values of the topocentric distance probability density. By increasing the number of generated sample orbits ($10 \rightarrow 200 \rightarrow n$), an unbiased phase-space region of possible orbits is found. Each sample orbit is assigned a weight, which describes how well it explains the observations. In addition to the accuracy requirement, the relative weights $\Delta\chi^2$ of trial orbits can also be multiplied with an informative a priori p.d.f. (Eq. 5). As a simple example, consider a situation where an object is considered to be an NEO, but IEO orbits cannot be ruled out. It has been estimated that the number of IEOs is approximately equal to 2% of the number of NEOs (Bottke et al. 2002a). The weights of acceptable IEO orbits could thus be multiplied with 0.02, whereas the weights of acceptable NEO orbits could be multiplied with unity. The orbital solution could now be used to more realistically assess which type of object the observations correspond to (cf. Paper I). In identification, the relative weights are typically ignored (although simple a priori p.d.f.s are used, see, e.g., Paper VI), and the distribution merely shows the extent of acceptable solutions in the orbital-element phase space.

A stepwise version of Ranging was developed in Paper II, and the techniques required for the full n -body problem were developed in Paper IV. In stepwise Ranging, all the data are not treated immediately, but the amount of data increases step by step. Simultaneously, the topocentric distance intervals are adjusted iteratively. As compared to conventional Ranging, its stepwise version requires fewer trial orbits to detect constrained orbital-element p.d.f.s. Whereas the trial orbit has so far been computed from the two heliocentric positions with methods utilizing the two-body approximation, a simplex optimization method for making the n -body corrections was presented in Paper V (for the generally applicable simplex method, see Nelder & Mead 1965).

When enough data is available to assume that a linearization of the inverse problem is acceptable, the well-known least-squares method with linearized covariances (LSL; see, e.g., Muinonen & Bowell 1993) is applicable. In addition to

conventional LSL, the incomplete and/or partial differential correction methods are also used. In incomplete differential correction, one or more of the orbital elements are fixed when correcting the rest. When using partial steps, the elements are not corrected by the correction computed, but only, say, a tenth of the correction is used in each element.

For moderate data leading to non-Gaussian constrained orbital-element p.d.f.s, Ranging typically requires an impractical amount of trial orbits, whereas the orbital uncertainty estimates obtained by LSL are misleading due to the Gaussian assumption. Therefore, the six-dimensional phase-space volumes-of-variation method (VoV; Paper III) was developed. The six-dimensional VoV method generalizes the one-dimensional LOV (see, e.g., Milani 1999) method. In VoV, one or more orbital elements are first selected as mapping elements. The mapping intervals are defined as the standard deviations, which are computed for the mapping elements with global, complete LSL, multiplied by constants iteratively adjusted to ensure that the relevant phase-space volume is treated. Then, the mapping parameters are systematically stepped through using a predefined number of steps. For each step, a local LSL solution is computed using incomplete differential correction for the remaining, “free” elements. Together with the interval(s) of the mapping parameter(s), the 5×5 or smaller covariance matrices define a six-dimensional hypervolume. Finally, the six-dimensional hypervolume is randomly sampled in Monte Carlo fashion. Similarly as in Ranging, acceptable trial orbits have to reproduce the observed positions with a given accuracy and, optionally, be accepted by the informative a priori p.d.f.

For any amount of data, acceptable single-point orbital solutions are obtained through a six-dimensional simplex optimization procedure in the orbital-element phase space, when a robust method not requiring partial derivatives is required (Paper V). However, the uncertainty of the simplex solution remains unknown.

A useful phenomenon for the classification of different orbital inverse problems—the stepwise evolution of the orbital-element uncertainty with increasing observational time span—was discovered by means of the rigorous, statistical inversion methods (Virtanen et al. 2005, see also Paper III). As seen in Figs. 3–5 of Paper III, the evolution of the orbital uncertainties as a function of the observational time span can be divided into three different regions. Typical for the first region are scarce astrometric data sets (two to, say, tens of observations) spanning less than a few hours (NEOs), less than a few days (MBOs), or less than a few months (TNOs) which result in wide, non-Gaussian orbital-element p.d.f.s. The second region—the so-called phase-transition region—typically consists of moderate data sets spanning several hours (NEOs), few days (MBOs), or a few months (TNOs) which typically result in constrained, nearly-Gaussian orbital-element p.d.f.s. The third region is typically reached when the observational time span is more than a

few weeks for NEOs, several months for MBOs, and several years or even tens of years for TNOs. Typical for the third region are orbital-element p.d.f.s that fairly accurately resemble the Gaussian distribution.

4 Identification

4.1 Theory

The foremost goal of all the following developments is to find all correct linkages in the input data. The orbit acceptably linking two or more data sets has to result in $O - C$ residuals similar to the assumed observational uncertainty. As shown through simulations in Paper II, the best-fit orbit of erroneous linkages typically has a lower $O - C$ residual root mean square (rms) value than the worst fit orbit of the correct linkages. A linking method aiming at a 100% sensitivity therefore cannot rule out one of two mutually exclusive candidate linkages based on the orbital fit, if both are acceptable in terms of their residuals. The philosophy behind the following developments is to start with all imaginable $\binom{n}{k}$ k -linkages, where n is the number of observation sets included, and remove candidate linkages that do not satisfy the conditions for an acceptable linkage by a stepwise application of different filters.

It is generally impossible to solve the identification problem by educated guesses or direct trial-and-error methods. Particularly as $n \rightarrow \infty$ the number of combinations explodes (Paper II) and alternative methods are called for.

The first task while searching for linkages between observation sets is to minimize the number of candidate linkages to be studied in depth. Let p_{pA} and p_{pB} correspond to the orbital-element a posteriori p.d.f.s (Eq. 4 or Eq. 5), which are based on the astrometry in observation sets A and B, respectively. Assuming that the sets are independent, the probability for set A (B) residing in the phase-space volume V_B (V_A) of object B (A) is

$$\begin{aligned} P(\mathbf{P}_A \in V_B) &= \int_{V_B} d\mathbf{P} p_{pA}(\mathbf{P}), \\ P(\mathbf{P}_B \in V_A) &= \int_{V_A} d\mathbf{P} p_{pB}(\mathbf{P}). \end{aligned} \quad (9)$$

The main significance of these probabilities of overlap is as follows: if it is possible to certify that

$$P(\mathbf{P}_A \in V_B) \approx 0 \quad \wedge \quad P(\mathbf{P}_B \in V_A) \approx 0, \quad (10)$$

the pair can be removed from the list of candidate linkages. Although orbital elements are used as the variable set in Eqs. (9) and (10), the removal of candidate linkages can also be based on any other variable set computed from the orbital elements using Eq. (6).

For nonzero overlapping p.d.f.s, the next step is to produce the orbital-element p.d.f. that is the product of the two separate p.d.f.s, with the assumption that the objects are the same so that one of the p.d.f.s plays the role of an a priori p.d.f. of

the other,

$$\tilde{p}_{\text{pAB}}(\mathbf{P}) \propto p_{\text{pA}}(\mathbf{P})p_{\text{pB}}(\mathbf{P}). \quad (11)$$

The Bayesian approach allows additional information to be formally present in the identification process. Let V_0 be the non-vanishing probability regime in the phase space covering all known asteroids (compare with the non-vanishing probability regime in the phase space containing all known TNOs in Virtanen et al. 2003). After proper normalization, it is possible to compute the probability of overlap with the phase-space volume V_0 of all known objects,

$$\tilde{P}(\mathbf{P}_{\text{AB}} \in V_0) = \int_{V_0} d\mathbf{P} \tilde{p}_{\text{pAB}}(\mathbf{P}), \quad (12)$$

If the probability is vanishingly small, the pair can be removed from the list of candidate linkages. However, this step is subject to iteration as it is not desirable to throw away new kinds of objects.

The probability of overlap given by Eq. (12) allows us to give a probability score P_C for any configuration C consisting of L_C linkages:

$$P_C = \sum_{l=1}^{L_C} \tilde{P}_l(\mathbf{P}_{\text{AB}} \in V_0), \quad (13)$$

where $C = 0, 1, 2, 3, \dots, C_{\text{tot}}$ and C_{tot} denotes the total number of configurations arising from the given linking problem.

The final result is an ordered list of configurations given, for example, by the following finite sequence K :

$$K = \{C_6, C_{12}, C_{200}, \dots, C_3\}. \quad (14)$$

In the case of numerous alternative configurations, the final derivation of the correct linkages and identifications is carried out via additional (new or archive) observations.

4.2 Numerical methods

The linking methods developed can each be divided into two different main filters. The first main filter discards the bulk of the $\binom{n}{k}$ candidate k -linkages using a loglinear algorithm. The loglinear computational complexity is obtained by using data structures called red-black binary search trees (hereafter RB trees). The second main filter attempts to find an orbit which reproduces the astrometry with $O-C$ residuals similar to the estimated observational uncertainty. If an acceptable orbit is found, it proves that the k sets of astrometry can be linked.

4.2.1 Red-black binary tree

The red-black binary search tree is a tree-like data structure which is guaranteed to stay approximately balanced in basic dynamic-set operations such as insertion, deletion, and search (for an introduction to various data structures, see, e.g., Cormen et al. 2003). Binary trees are data structures with up to two child nodes. The search key for the left child node is lower than the search key for the parent node, whereas the search key for the right child node is larger than the search key for the parent node. In general, dynamic-set operations on binary trees have a computational complexity of $\mathcal{O}(h)$, where h is the height of the tree. The depth of a node is the length of the downward path from the root to the node in question, and the height h is equal to the largest depth of the tree (see Fig. 3). A

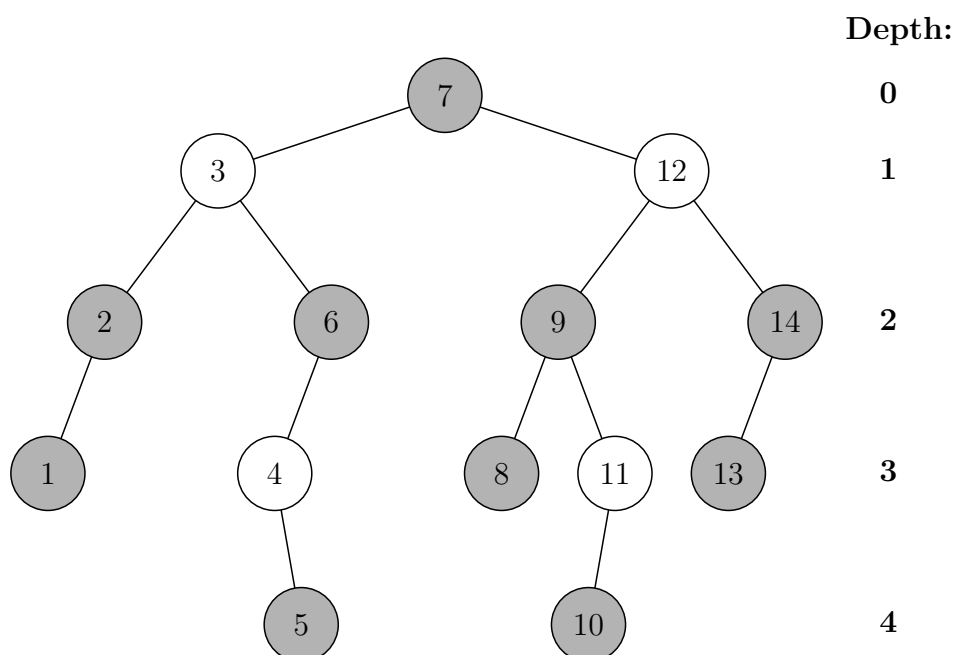


Figure 3: An example of a red-black binary tree. The search keys are specified as integer numbers within the nodes. The shading refers to black nodes, whereas the non-shaded nodes are red.

self-balancing binary tree tries to keep its height as small as possible at all times. In a complete binary tree, each internal node has exactly two children, and each leaf node has the same depth. The height of a complete binary tree is exactly $\log_2(n + 1) - 1$, where n is the number of nodes in the tree. That is, the height is $\mathcal{O}(\log n)$. It can be proven that the height h of a balanced binary tree is also $\mathcal{O}(\log n)$ (see, e.g., Cormen et al. 2003). The computational complexity of the dynamic-set operations for a balanced tree is thus guaranteed to be $\mathcal{O}(\log n)$.

For RB trees, the approximate balance means that the longest downward path from the root to a leaf node is less than twice as long as the shortest path from the root to a leaf node. The RB tree is kept in approximate balance by adding an extra bit of information to each node, the so-called color bit, and by fulfilling the following conditions:

1. Every node is either red or black.
2. The root node is black.
3. Every leaf node is black.
4. A red node's children are both black.
5. All paths from a given node to descendant leaf nodes contain an equal number of black nodes.

If the RB tree does not fulfill the conditions after a dynamic-set operation on a given node, a limited number of rotations depending on the colors of the node in question and the surrounding nodes as well as on their mutual relationships will restore the conditions. Because an RB tree is always approximately balanced, it can be proven that the computational complexity of the required rotations is $\mathcal{O}(\log n)$. Note that the rotations add a constant cost to each insertion and deletion operation as compared to a conventional, randomly built binary search tree.

4.2.2 Finding candidate linkages

The generally applicable multiple-address-comparison (MAC) method developed for the first main filter is based on the contents of Eq. (10), which states that almost zero overlapping probability densities computed for the orbital-elements or any spin-off variables based on the orbital elements (hereafter collectively referred to as the comparison variables) indicate that a candidate linkage can be discarded. Whereas the true orbital-element p.d.f. for an asteroid is continuous and includes the complete volume of physically acceptable values, the sampled p.d.f. covers a volume including a certain fraction, e.g., 99.9999%, of the total probability mass. Therefore, acceptable sample orbits cover a limited volume in the six-dimensional orbital-element phase space, the so-called nonzero probability density, whereas the probability mass in the remaining orbital-element phase space is assumed to be zero. Instead of using the rigorous weight for each sample orbit defined by Eq. (4) or Eq. (5), we have only used the extent of the p.d.f. If the sampled comparison-variable p.d.f.s for two or more different sets of astrometry overlap, the sets form a candidate linkage.

The type of comparison variables chosen depends on the characteristics of the linking task. For the short-term problem, we usually use geocentric ephemerides which are computed for, say, three common epochs (ephemeris-space MAC, or eMAC; see Paper II), because the ephemerides preserve the accuracy of the transverse sky-plane coordinates observed for a limited period after the observation dates. For the long-term problem, nearly constant integrals of motion such as Keplerian orbital elements are preferable (orbital-element-space MAC, or oMAC, see Paper VI). Note that the number of comparison variables chosen (k) varies. In MAC, the k -dimensional comparison-variable space is first discretized. Using the bin sizes and the total intervals for the variable, an individual *address* I (in practice, an integer) can be computed for each set of k comparison variables. Each dimension of the k -dimensional comparison-variable space is first discretized into m_d ($d = 1, 2, \dots, k$) intervals. Let the k indices of a certain bin in the discretized comparison-variable space be $i_d > 0$ ($d = 1, 2, \dots, k$). That given bin then obtains an address given by the single integer

$$I = 1 + \sum_{j=1}^k (i_j - 1) \prod_{l=1}^{j-1} m_l. \quad (15)$$

Assuming a master set with n subsets of astrometry and m orbits being used to sample the orbital-element p.d.f. resulting from the astrometry, the computational complexity of the addressing is linear, that is, $\mathcal{O}(nm)$.

Next we search for identical addresses obtained from two or more data sets. If an equal address is found, it implies a potential linkage as the comparison variables are similar although not necessarily identical. The search for equal addresses is efficiently performed using tree-like data structures. Whereas randomly built binary trees have the minimum cost per operation, we cannot assure that the data, that is, the addresses, are inserted in a completely random order. Unless the values are inserted in random order, the computational complexity for dynamic-set operations on a randomly built binary tree could, in the worst-case scenario, be linear. Systematic trends may arise in the line of input addresses, because the last element of the comparison-variable vector is most influential for the actual value of the address. For constrained comparison-variable p.d.f.s, all addresses are thus essentially similar, and the input addresses would come in “clumps” rather than randomly distributed. Note that Paper II contains a related discussion on the reason for the varying efficiency of the then-used MAC algorithm. To guarantee the optimum computational complexity for the dynamic-set operations, we have chosen to use an augmented data structure with the RB tree as the underlying data structure.

In the MAC algorithm, the addresses are used as search keys for the nodes of the RB tree (hereafter the address tree), and each node contains another data struc-

ture, for example, a list, which in turn contains the identifier of the original data set (Fig. 4). As the insertion is guaranteed to have a logarithmic computational complexity, the insertion of nm addresses will have a computational complexity of $\mathcal{O}(nm \log nm)$. When all addresses have been inserted to the address tree, the MAC algorithm has essentially performed the first filtering. Consider the i th node N_i of an address tree which includes N_{addr} different addresses, or nodes. The l_i data sets, whose identifiers are found in node N_i , have obtained similar values for the comparison variables, and therefore constitute, for example, $\binom{l_i}{2}$ candidate 2-linkages or $\binom{l_i}{3}$ candidate 3-linkages.

The next step depends on the methods used in the second main filter (Sect. 4.2.3). The operation of the MAC filter ends here, if candidate linkages are further analyzed using methods requiring the information contained in the addresses (oMAC; Paper VI). However, if the information contained in the addresses is not used (eMAC), the whole address tree is traversed and all $\sum_{i=1}^{N_{\text{addr}}} \binom{l_i}{k}$ candidate k -linkages are extracted (cf. Paper II). When $l_{\text{max}} > k$, the time complexity of the process is $\mathcal{O}(N_{\text{addr}} l_{\text{max}}^k)$, where l_{max} is the maximum number of sets having the same address. Even though l_{max}^k apparently destroys the scalability of the method, the size of l_{max} can be reduced by simultaneously increasing both the resolution of the discretization and the number of sample orbits m . Note, however, that to some extent, l_{max} is defined by the data. If, for example, ten sets of astrometry of the same asteroid are analyzed, l_{max} cannot be forced to be smaller than ten. Similarly, if, say seven, different asteroids can be (erroneously!) linked assuming a realistic astrometric uncertainty, l_{max} cannot be forced to be smaller than seven. However, in all practical problems so far analyzed with eMAC, the size of l_{max} has not been a problem. To make sure that every linkage is extracted only once, the pairs of identifiers for linked data sets are inserted into another RB tree, the so-called linkage tree (Fig. 5). The insertion process automatically rejects the insertion, if a linkage has already been inserted to the tree. Building the linkage tree has a computational complexity of $\mathcal{O}(N_{\text{addr}} l_{\text{max}}^k \log N_{k\text{-link}})$, $N_{k\text{-link}}$ being the number of k -linkages found. The extraction of the $N_{k\text{-link}}$ k -linkages from the linkage tree is a linear process, that is, it has a computational complexity of $\mathcal{O}(N_{k\text{-link}})$.

Note that the MAC algorithm does not specifically compare the p.d.f.s stemming from two different observation sets: it only organizes the data so that the linkages can be picked up. Based on empirical comparisons, the loglinear method requires a similar computational effort as the simpler quadratic method (Paper II) when including up to hundreds of data sets. For more numerous data sets the new method is clearly faster as expected.

In problems where the Gaussian assumption is valid for at least one of the astrometric observation sets, the $\Delta\chi^2$ metric (cf. Eq. 8) is used to find potential linkages. If covariance analysis through linearization is applicable to both sets,

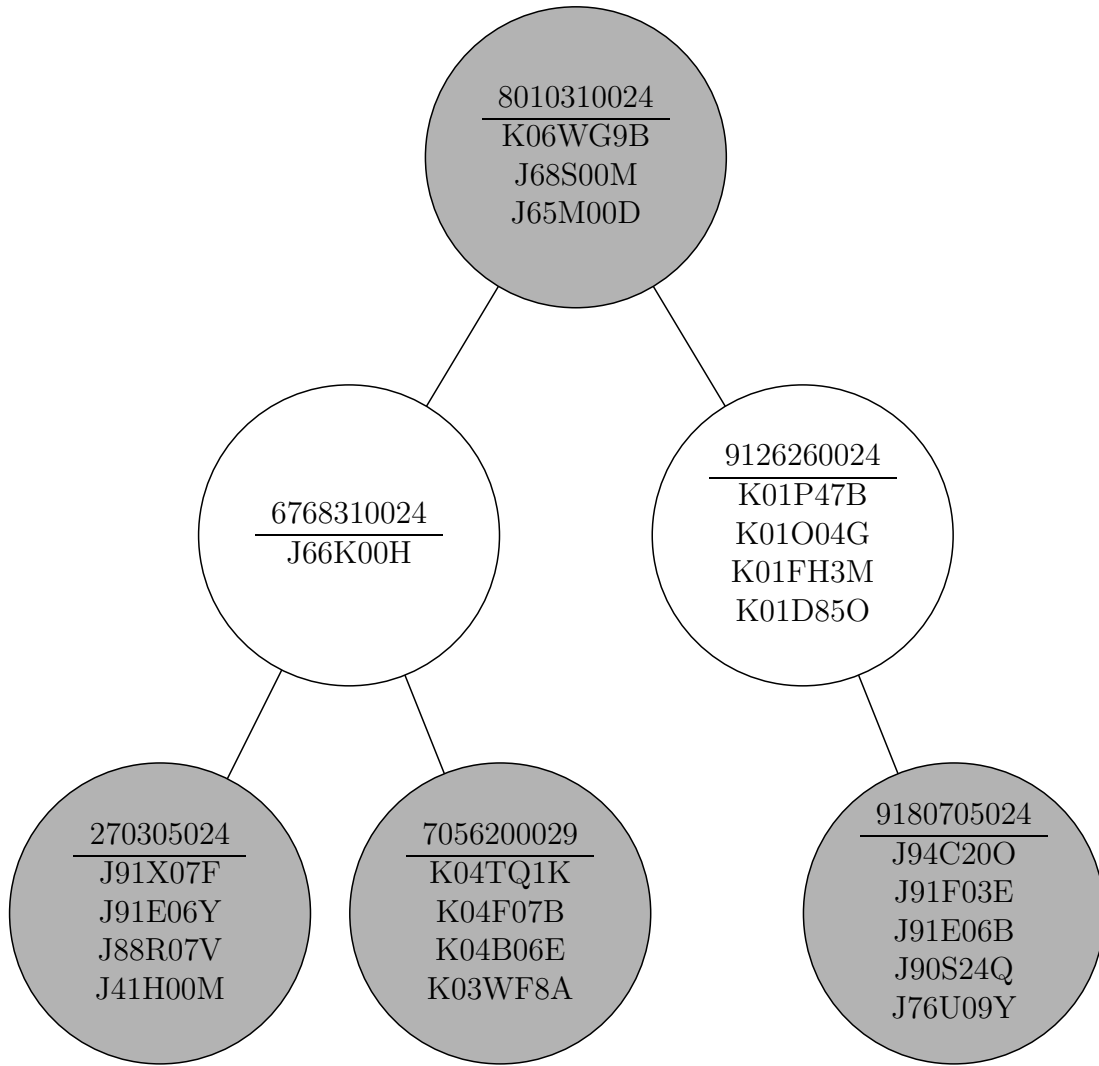


Figure 4: An example of an address tree. The addresses are used as search keys, and the identifiers of the observation sets resulting in the addresses are included in another data structure within each node.

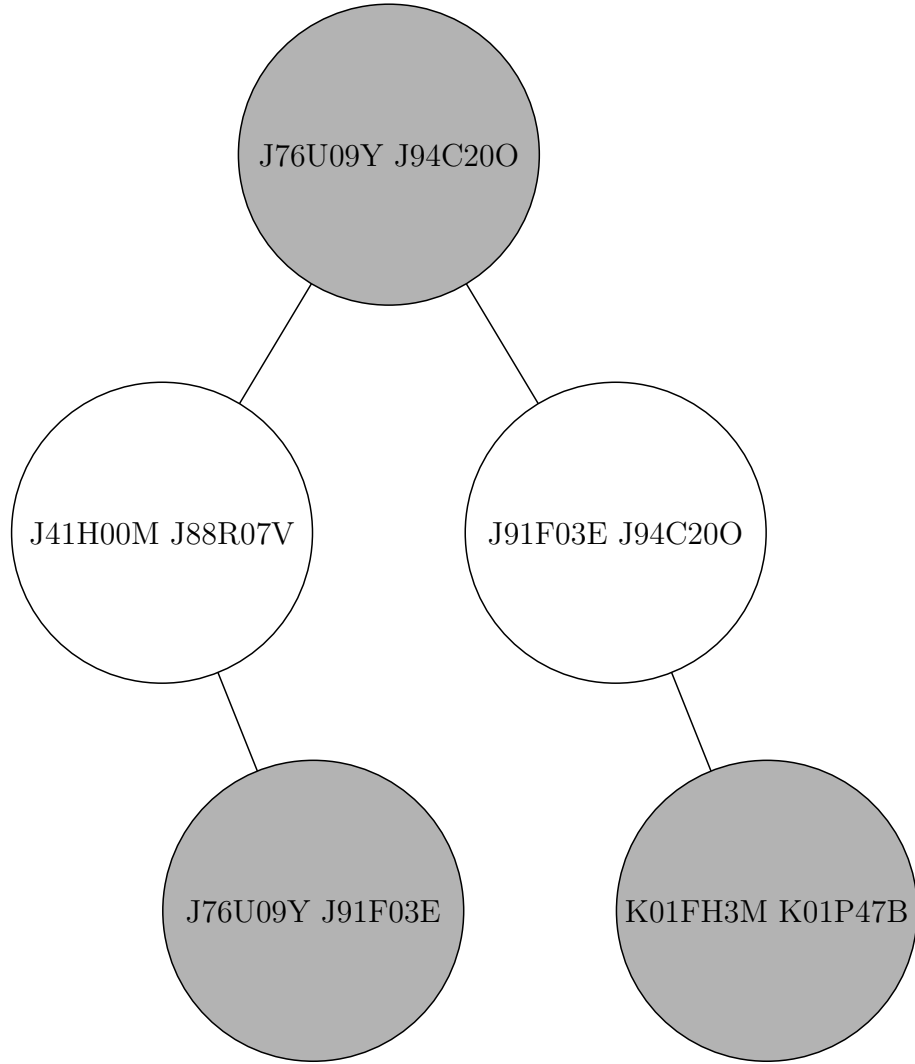


Figure 5: An example of a linkage tree. The identifiers of the observation sets that form a candidate linkage are used as search keys. To guarantee that each linkage is only inserted once, the identifiers are always sorted in ascending order.

the uncertainty ellipsoids defined by the covariance matrices need to overlap at, e.g., the $3\text{-}\sigma$ level to qualify as an interesting couple (cf. Milani et al. 2000). If the covariance analysis is applicable to only one of the sets, e.g., identifying single-night sets of astrometry with numbered asteroids, the orbital-element covariances are propagated to the ephemeris space at the observation date(s) and the $\Delta\chi^2$ value between the ephemerides and the observations is utilized in the search for candidate identifications. When comparing a rigorous sampled p.d.f. and a Gaussian p.d.f. defined by the covariance matrix, the $\Delta\chi^2$ value is computed for each sample orbit with respect to the nominal least-squares orbit and its covariance to find candidate linkages.

Particularly in long-term linking, the n -body propagation of the orbital elements from the inversion epoch t_{inv} to a common comparison epoch t_{comp} can lead to non-Gaussian p.d.f.s, which may in turn lead to correct candidate linkages being erroneously discarded (cf. Milani et al. 2000). To increase the sensitivity of the first main filter, the uncertainty ellipsoids defined by the covariance matrices should usually be sampled even when the separate orbital inversion problems can be linearized. The search for overlapping sampled uncertainty ellipsoids can then be done using the MAC method described above.

4.2.3 Verifying candidate linkages

Although the theory for the verification of candidate linkages is outlined by Eqs. (11)–(14), it has not yet been accurately implemented in numerical methods. For example, the product of two separate orbital-element p.d.f.s given by Eq. (11) is efficiently computed by combining the astrometry corresponding to a candidate linkage, and solving the orbital inverse problem for the combined astrometry. Considering Eqs. (13) and (14), it is not clear whether a few linkages leading to extraordinary small $O - C$ residuals are more important than a larger number of linkages with ordinary residuals. In both cases, the probability scores may be similar. To date, we have only used an approach resembling the theory outlined by Eqs. (13) and (14) when choosing between a few alternative linkages (Paper III).

By using the classical initial orbit determination methods such as Gauss’ method when solving Eq. (11), one may erroneously discard correct identifications, because a single orbit reproducing the astrometry cannot be found. Therefore, various sampling methods are used in the second filter. For short-term linkages, the uncertainty of orbital elements computed from the combined data set does not, typically, reach the phase-transition region (see Sect. 3.2). Ranging is therefore suitable for the search of the orbit linking the astrometry. When the same initial parameters are used, but the amount of data increases, the fraction of trial orbits accepted decreases. The reason for the decreasing fraction of trial orbits accepted is that the

phase-space volume of acceptable orbits decreases with an increasing amount of data, whereas the phase-space volume of trial orbits stays constant. If the sampling intervals are adjusted iteratively while stepwise increasing the amount of data, the fraction of accepted trial orbits does not decrease too much. The maximum number of trial orbits allowed can therefore be reduced by orders of magnitude, which in turn means that erroneous linkages, for which acceptable orbits cannot be found, can be discarded more rapidly. The stepwise version of Ranging is presented in Paper II, and the empirical results verify that it performs as expected.

Although there exist cases where it is practical to use Ranging when searching for the orbit linking observation sets obtained in different apparitions (see, e.g., Virtanen et al. 2003), Ranging is not the optimum tool in general. For long-term linkages, the phase-space volume of acceptable orbits is usually too constrained to be detected by a sampling method without a priori knowledge of approximate sampling intervals. However, if the first filter has been working in the orbital-element phase-space, one can instead make use of the addresses and their information. The indices i_d of the bin in the orbital-element phase-space can be obtained from the address with the recurrence relation

$$i_d = (1 - \delta_{1d}) + \text{int} \left[\frac{I - \sum_{j=d+1}^k (i_j - 1) \prod_{l=1}^{j-1} m_l}{\prod_{j=1}^{d-1} m_j} \right], \quad (16)$$

where δ_{ij} is the Kronecker symbol. Using the indices i_d and the bin sizes, the intervals defining the relevant volume in the orbital-element phase-space can be computed. As the information in the address defines at least a fraction of the volume in the orbital-element phase-space in which the orbital-element p.d.f.s overlap, a set of orbital elements, providing a reasonable fit to the observations, can be obtained via random sampling in that volume. To obtain anything closely resembling the maximum-likelihood orbit, an impractical amount of sample orbits would be required. Instead, the best sampling orbit can be further optimized by using the least-squares method. To make sure that the orbital solution for correct linkages converges, one can make partial and/or incomplete differential corrections.

As mentioned in Sect. 4.2.2, extracting linkages from the address tree (Fig. 4) is not a necessity for proceeding to the second main filter. Instead, the random sampling described above can be performed simultaneously for all observation sets sharing the same address, that is, are found in the same node. The sample orbits collect all those observation sets that can possibly be linked. For example, consider a node with 300 different observation sets. The number of different candidate 3-linkages is thus $\binom{300}{3} = 4,455,100$. If the phase-space volume defined by the address were to be sampled separately with, say, 5,000 orbits for each of the 4,455,100 3-linkages, the impractical amount of 22,275,500,000 sample orbits would be needed for a single node. However, if all observation sets are treated simultaneously, and only the relevant 3-linkages are extracted from the node, both the

number of sample orbits (5,000) and the number of 3-linkages explicitly analyzed (typically a small fraction of the 4,455,100) are kept within practical limits.

The dynamical model to be used during the second main filter depends on the identification problem. For short-term identification, the Keplerian two-body model taking into account the gravitation by the Sun is typically adequate whereas, for long-term identification, the n -body model taking into account the gravitation by other relevant solar-system bodies in addition to the Sun is the norm. Note that the choice of the dynamical model usually becomes relevant only in the very last filter, when a high accuracy is typically called for.

For methods based on a linearized orbital solution such as the ones described in the second last paragraph of Sect. 4.2.2, the orbits are typically accurate to the point that the verification of candidate linkages can be performed using a differential correction method starting with the existing orbit(s).

4.3 Selected results

Granvik et al. (2005a) applied the short-term identification method to single-night asteroid astrometry obtained with ESO's Very Large Telescope (VLT). The short-term method found at least one linkage to all but 103 of the 532 detections, and four or more nightly sets of astrometry had to be linked to produce only unambiguous linkages (Fig. 6). In Paper III, the VLT data was combined to astrometry obtained with the Canada-France-Hawaii Telescope (CFHT) and the Spitzer space telescope. The latter is operating in the infrared wavelength region. Due to nearly-simultaneous observations obtained from substantially differing locations—the distance from Spitzer to the Earth was ~ 0.07 AU during the campaign—a substantial parallax was present in the data. However, the short-term method successfully linked the astrometry despite the parallax (Fig. 7).

Recently, a survey was started to locate 3-linkages among the $\sim 50,000$ provisionally designated single-apparition sets of astrometry spanning less than 48 hours. As of September 21, 2007, the long-term identification method has found 54,002 3-linkages fulfilling the criterion that the orbital fit of acceptable linkages must have an $O - C$ residual rms of less than $3''$. Some 8,000 3-linkages have an rms value smaller than $1''$. Although most of the detected linkages have MBO-type orbits, 381 3-linkages with NEO-type orbits have also been found (21 have rms values less than $1''$; Fig. 8).

4.4 General remarks

Due to the statistical nature of the methods described above, they cannot, theoretically, reach a 100% sensitivity. However, in simulations, the methods typically find practically all correct linkages. One reason for missing correct linkages is the

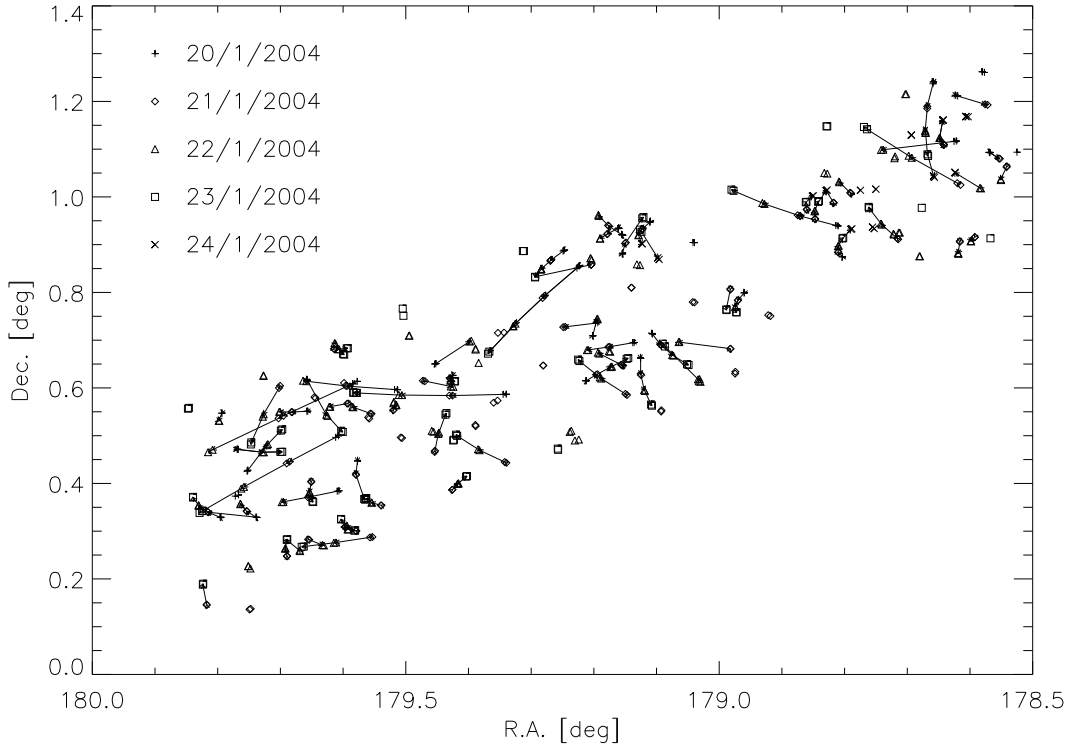


Figure 6: Linkages among 532 asteroid detections at $V \lesssim 26$ mag spread over five nights obtained with the VLT in January 2004. The short-term linking method found 76 2-linkages between altogether 429 detections. The linkages are indicated with lines.

limited number of orbits used to sample the orbital-element p.d.f. It happens that the “true” address, computed for the “true” values for the comparison variables, which in turn can be defined as the maximum-likelihood values that would be obtained for an infinite amount of data, is not included in the set of addresses corresponding to a scarce data set. On one hand, when searching for linkages among scarce data sets, the uncertainties will result in wide address distributions, and equal addresses will typically be found in the address space surrounding the “true” address, at least for correct linkages. The properly treated uncertainty therefore acts as a helping factor in the search for linkages. On the other hand, if one of several data sets referring to the same asteroid contains a substantially larger amount of data as compared to the other sets, the extensive data set may lead to only the “true” address, whereas the “true” address may escape the other sets. All correct linkages would therefore not be found. However, in cases like the second one, the choice of the identification method has typically failed, as the scarce observation sets should have been identified by using linear methods such as the ones outlined above.

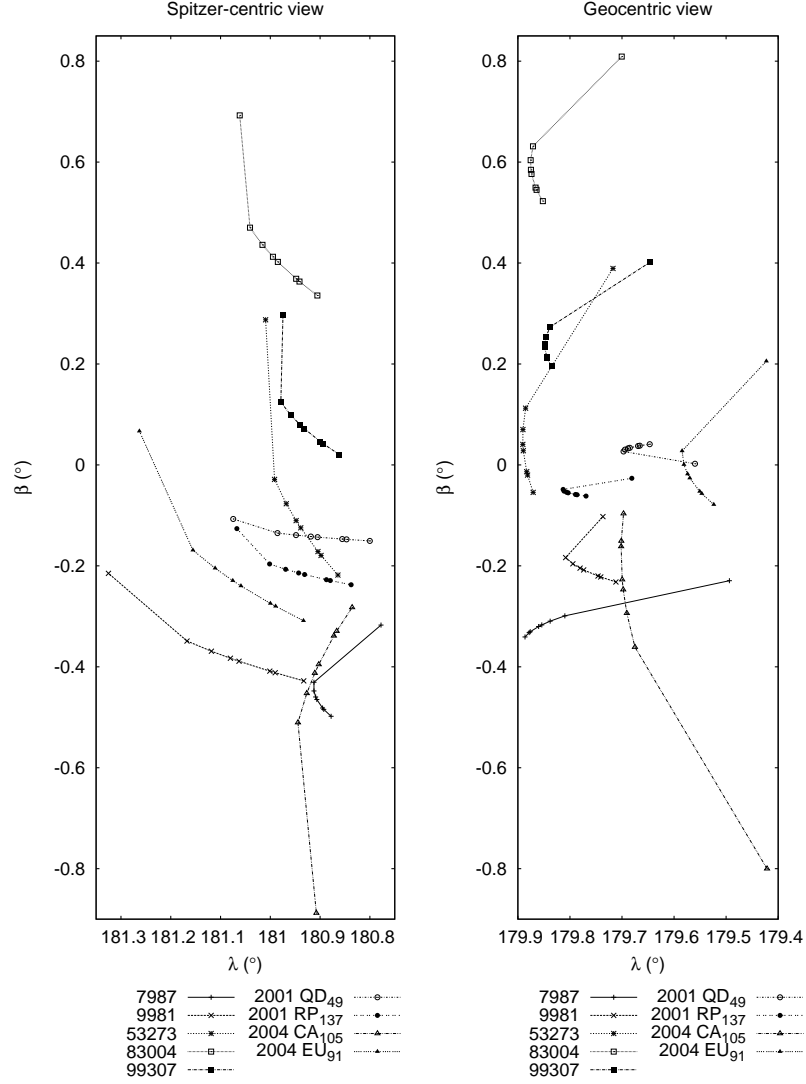


Figure 7: Ephemerides for nine identified and also independently correctly linked Spitzer objects as seen by a Spitzer-centric observer (left) and by a geocentric observer (right). The computed positions correspond to approximate real observation dates by different telescopes in January 2004 (UTC): 20.289 (VLT), 21.124 (Spitzer), 21.289 (VLT), 22.289 (VLT), 22.589 (CFHT), 23.289 (VLT), 24.289 (VLT), and 30.589 (CFHT). The $\gtrsim 1^\circ$ angular separation between the Spitzer spacecraft and Earth-bound observatories as seen from the MBOs lead to strikingly different motions and relative locations depending on the observer location. Note that the lines do not correspond to the precise paths of the objects, but merely connect simulated positions of the same object to help guide the eye.

According to extensive simulations (see, e.g., Kubica et al. 2007), the number

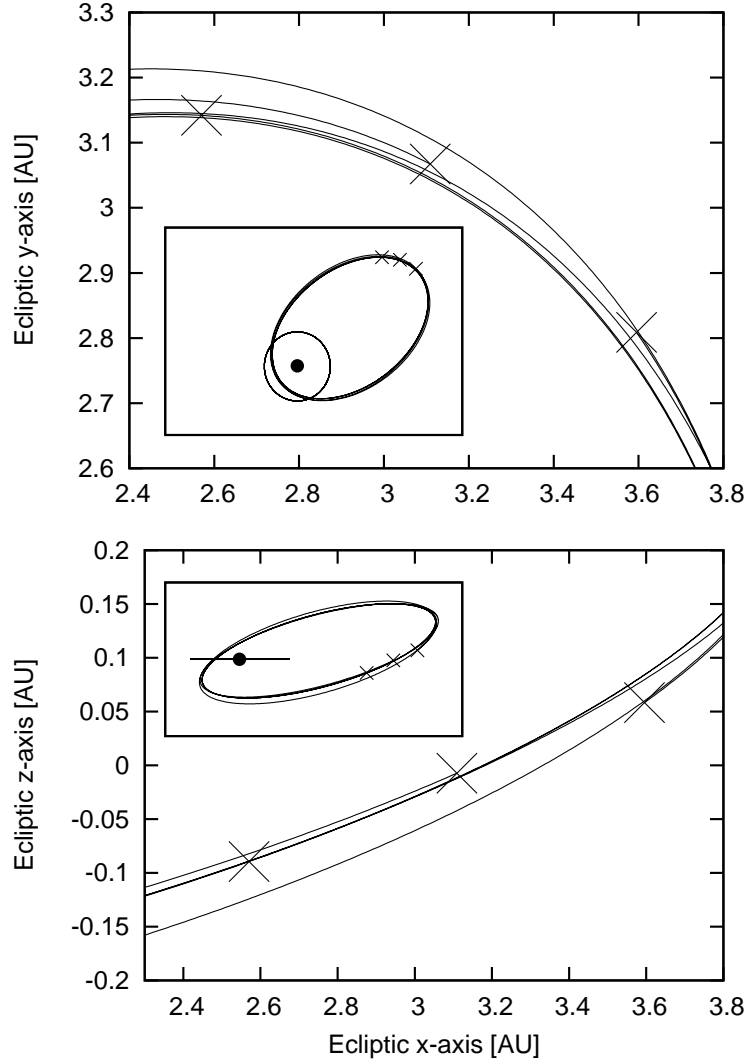


Figure 8: An example of a 3-linkage found between single-night observation sets from different apparitions. The observations are linked with a single NEO-type orbit over a time span of approximately 21 years with an rms error of $0.48''$ in R.A. and $0.98''$ in Dec. Starting from the left, the provisional designations for the observation sets are 1996 WS₃, 1983 VV₆, and 2004 TQ₃₆₃. The Sun and the Earth's orbit are also shown. Note that whereas this particular linkage is not necessarily correct, it proves that the long-term linking method is capable of finding realistic linkages over long time intervals using extremely scarce data.

of false-positive detections for Pan-STARRS is equal to the number of true detections on the ecliptic for a $5\text{-}\sigma$ detection limit, which means that only signals five times stronger than the standard deviation of the background noise are accepted.

For regions off the ecliptic, the ratio between true and false-positive detections decreases dramatically. The handling of the false-positive detections in the linking process can therefore be challenging. As stated in the first paragraph of Sect. 4.1, the methods developed do not rule out acceptable linkages. The false-positive detections will eventually either show up as outliers, or remain unidentified, but correct linkages will not be lost due to the presence of false-positive detections. On one hand, the problem thus appears to be an observational one: How many follow-up observations have to be obtained and for how long, until it can be ruled out that an orbit would be based on erroneously linked data? In both simulations and applications to real data (Papers II and III), erroneous or mutually exclusive linkages cannot be found after five nights of observations within a time span of a week or so. Note, however, that these results have been obtained for a density of detections somewhat smaller than what is expected for Pan-STARRS. On the other hand, the problem can also be treated as a computational one: For how long is it possible to carry along unverified linkages given limited computational resources? A straightforward answer cannot be given, because it depends on the computation infrastructure available.

Whereas identification methods based on statistical orbital inversion might not be the fastest ones, the other methods face different types of problems stemming from the approximations and approaches used. The types of problems encountered are connected to substantial parallaxes, numerous asteroids in a limited area, scarce data sets, long linking intervals, and foremost, massive amounts of data. Substantial parallaxes are challenging, if not impossible, for methods using polynomial extrapolation of observed positions to compute approximate ephemerides (Kubica et al. 2007), because the topocentric distance r is not treated. Substantial parallaxes are also challenging for the short-term identification method by Milani et al. (2005a), because r and the radial velocity \dot{r} are only sampled for the first attributable. The acceptable (r, \dot{r}) -pairs are used to locate linkages by searching for acceptable solutions when combining an (r, \dot{r}) -pair with the second attributable. As long as the parallax can be assumed negligible, the acceptable (r, \dot{r}) -pairs are often roughly similar at the dates of both attributables. However, for substantial parallaxes, the difference between acceptable (r, \dot{r}) -pairs at the two dates can become too large to allow correct linkages to be found. As the present statistical methods search for linkages using complete orbital solutions, r is properly treated for all sets. Parallaxes will therefore not pose a problem for identification (Paper III). Extensive amounts of asteroids in a limited area will typically lead to confusion, and methods based on simplifying assumptions (e.g., Kristensen 2007) can become challenging to manage as correct linkages may be erroneously discarded. The statistical orbital inversion methods are the only ones capable of producing reliable estimates for the orbital uncertainties stemming from scarce data sets, which

is particularly important for the long-term linking. In addition to the short-term and long-term identification methods described in the present thesis, only Kubica et al. (2007) have so far presented a loglinear identification method applicable for the future massive surveys.

5 Summary of papers

5.1 Paper I

Transneptunian Object Ephemeris Service (TNOEPH)

The paper presents a Ranging-based web service to aid the identification of precovery observations of TNOs and the planning of follow-up observations of TNOs. First, using TNO astrometry and an astrometric uncertainty estimate supplied by the user, the orbital-inverse problem is solved for the orbital-element p.d.f. Second, the orbital-element p.d.f. is used in the generation of topocentric ephemerides for a given date and observatory. In addition to a plot of the extent of the ephemeris p.d.f., the service also returns plots showing various orbital elements as functions of the predicted R.A. at the ephemeris date. Furthermore, the service also returns plots showing the extent of the ephemeris p.d.f.s for different classes of TNOs. Note that the service can also be used when searching for the orbit linking separate sets of astrometry. The service successfully returns ephemerides, if an orbital solution exist for a combined set of astrometry.

5.2 Paper II

Asteroid identification at discovery

We present a Bayesian theory for the linking of asteroid astrometry, and develop a numerical method for the solution of all currently imaginable linking problems with astrometric data sets each containing more than one observation. The new method (for an early version of the method, see Granvik 2003) is optimized for the short-term linking of scarce astrometric data sets over time intervals of up to several months (for MBOs). For the first main filter, we develop the MAC method which is here used in ephemeris space. For the second main filter, the stepwise version of Ranging is developed. It discards erroneous linkages faster than conventional Ranging. The methods developed were successfully tested using numerous simulated single-night sets of astrometry. The successful application to single-night astrometry obtained with ESO's Very Large Telescope (VLT) is shortly reviewed (Granvik et al. 2005a). As far as I know, the methods presented describe the first complete solution to the short-term linking problem—including both the search for candidates and their verification through a linking orbit—published in a peer-reviewed journal.

5.3 Paper III

Linking Large-Parallax Spitzer-CFHT-VLT Astrometry of Asteroids

As a continuation to the work in Paper II and by Granvik et al. (2005a), the new short-term linking method was applied to scarce astrometry obtained nearly-simultaneously from ground-based and space-based observatories. Observations with the Spitzer infrared space telescope were made to obtain radiometric size estimates for small main-belt asteroids. Nearly simultaneously, follow-up observations were obtained with CFHT and VLT to reduce the detected objects' topocentric and heliocentric distance uncertainty as many of the detected objects were new discoveries. The comparatively large distance between the ground-based telescopes and the Spitzer spacecraft (~ 0.07 AU) led to a significant difference in the nearly-simultaneously obtained observed coordinates—exactly as planned in advance. Whereas the parallax can be utilized in orbital inversion to substantially reduce the uncertainty of the orbital elements, it makes the linking task, which precedes the final orbital inversion using all linked data sets, more complicated. As the linking method developed in Paper II is built upon rigorous orbital inversion methods, the parallax is automatically taken into account. Using simulated astrometry closely resembling the real data, we showed that the method can find practically all correct linkages between Spitzer astrometry and ground-based astrometry. Then we applied the method to the real astrometry, and found all the linkages already detected by the MPC and, in addition, a few previously hidden linkages. The heliocentric and topocentric distances (with exact uncertainties) to the asteroids detected by Spitzer were then estimated for the observation dates using Ranging, VoV, or LSL, where applicable. Simultaneously, we also estimated the phase angles and their uncertainties for the same objects and dates. From the final results, we derived an empirical rule of thumb for the decrease in orbital uncertainty that can be obtained from stereoscopic astrometry.

5.4 Paper IV

Asteroid orbits using phase-space volumes of variation

Whereas Ranging is optimized for scarce data and LSL is applicable for extensive data, the paper presents the six-dimensional phase-space volumes-of-variation method, a new Bayesian orbital-inversion method optimized for intermediate, or transitional data. Essentially, VoV is a six-dimensional generalization of the one-dimensional LOV method (for examples of different LOV methods, see Milani 1999, Muinonen 1996, Bowell et al. 1993). In VoV, local, incomplete least-squares solutions (including the incomplete covariances) along the ridge of the orbital-element p.d.f. are used as maps when sampling the p.d.f. in six dimensions. Note that in LOV, non-Gaussian features are properly treated in one-dimension, whereas VoV treats all six dimensions rigorously. As a demonstration, VoV is successfully applied to NEO, MBO, and TNO astrometry with varying observational time spans. The uncertainty estimates coincide with Ranging for data with a short observa-

tional time span and with LSL for data with a long observational time span. The phase transition in orbital uncertainty as a function of the observational time span and object type is also presented. The impact of observational cadence and amount of data is demonstrated for an MBO by the computation of the real evolution of the ephemeris uncertainty and its hypothetical evolution had additional observations not been obtained.

5.5 Paper V

Near-Earth-Object Identification Over Apparitions Using n -body Ranging

For the long-term linking of NEOs making close approaches to the Earth, Ranging was further developed by completely removing the two-body approximation from the analysis. In Ranging, the two-point boundary-value problem—the problem of finding the orbit that reproduces two Cartesian heliocentric positions—is usually solved using either the so-called Hansen’s continued fraction method (e.g., Dubyago 1961) or the p -iteration method by Herrick and Liu (e.g., Danby 1992). Both methods iteratively solve for a two-body orbit which reproduces the two heliocentric positions with desired precision. Even though the sample orbits have been compared with observed positions using n -body ephemerides where needed, the initial two-body approximation has so far remained in the final results. Here we present a new method, which starts with a two-body orbit computed using the continued fraction method or the p -iteration method, but uses the simplex algorithm (Nelder & Mead 1965) to include n -body perturbations to the solution of the two-point boundary-value problem. The simplex technique was initially developed for linking purposes, but it may also turn out to be valuable for the computation of precise impact probabilities, e.g., between the Earth and an NEO.

5.6 Paper VI

Asteroid identification over apparitions

Based on the theory and partly on some of the techniques put forward in Paper II, we present a new method for the search of long-term linkages among numerous scarce data sets. For the first main filter, that is, the MAC filter, we developed a new loglinear comparison algorithm. Applications to simulated astrometry indicates that the method is able to find 96% of the correct MBO 3-linkages and 92% of the correct NEO 3-linkages between data sets obtained during 13 years and each spanning approximately 24 hours, when using an informative a priori p.d.f. in the orbital inversion. According to early results from an ongoing survey to find linkages among the approximately 50,000 astrometric data sets spanning less than

two days, the new method had already found tens of realistic linkages at the time of the initial submission of the manuscript on September 4, 2007.

5.7 Author's contribution

For Paper I the author developed the web routines and plotting routines, as well as wrote the paper and generated the plots. For Papers II, III, V, and VI, the author developed most of the new numerical methods required. Furthermore, the author was responsible for the generation of simulated data and the numerical tests, for the application of the methods to real data, for writing the papers (except for Sect. 2 of Paper II which was a shared effort), and for making the plots.

For Paper IV, the author participated in the development and automation of the VoV method which is implemented as part of the Orb package. The author was also responsible for the generation of the final plots for the manuscript.

The numerical methods required for the analyses presented in Papers II–VI and some of the methods required for Paper I are included in the Orb orbit-computation software package written in Fortran 90/95 following the object-oriented programming paradigm (Decyk et al. 1997). The author initiated the development of the Orb package, and has since been the primary designer and developer of the software. J. Virtanen, T. Laakso, and K. Muinonen have also participated in the development. Excluding the empty lines, the continuously evolving Orb software package currently includes some 80,000 lines of code.

6 Conclusions and future prospects

The present thesis provides a complete theoretical solution to asteroid identification by using statistical orbital inversion methods. Loglinear numerical methods have been developed both for short-term and long-term identification of asteroids among numerous scarce data sets. Particularly, the hitherto unsolved long-term problem of finding linkages among scarce data sets obtained at different apparitions has been solved.

The fact that the methods described in the thesis have been able to detect almost 40 previously unknown asteroids in a data set containing the unidentified single-night sets obtained during a period of only three months proves that numerous new discoveries are waiting to be made among the archived sets of astrometry (Granvik et al. 2005b). Recently, a systematic survey to find linkages among provisionally designated observation sets spanning less than 48 hours was started (Paper VI). The survey utilizes the long-term identification method developed. In the future, identifications will be sought among all single-apparition objects including the unidentified single-night sets of moving-object astrometry archived by the MPC.

During the years, various commentators have claimed that statistical methods cannot be used to solve large-scale problems. In my mind, the present thesis and the continuously improving computer hardware proves the opposite. Whereas it is true that the orbit computation methods based on analytical approximations are often faster than the statistical methods, the loglinear identification methods developed show that the latter can be applied to large-scale problems. However, to keep the computational requirements on levels practically achievable, new techniques—not necessarily trivial or immediately apparent—such as those presented in this thesis, need to be developed and used.

The numerical identification methods presented do not currently utilize all the information available from the Bayesian orbital inversion approach. For example, the relative weights have been omitted, and only the extent of the nonzero p.d.f. has been used. In the future, the inclusion of the relative weights in the identification process should be studied in depth. The use of an informative a priori p.d.f. as outlined in the identification theory could become relevant when analyzing low signal-to-noise detections, a high fraction of which are false-positives.

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